REPORT DOCUMENTATION PAGE

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
	Technical Papers	

4. TITLE AND SUBTITLE		5a. CONTRACT NUMBER
		5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)	5d. PROJECT NUMBER
	2303
	5e. TASK NUMBER
	M2C8
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT
Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048	

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048	11. SPONSOR/MONITOR'S NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

1121 033

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Leilani Richardson
Unclassified	Unclassified	Unclassified	A		19b. TELEPHONE NUMBER (include area code) (661) 275-5015

2303/1208 TP-FY99-0110

✓ Spreadsheet
✓ DTS

MEMORANDUM FOR PRR (Contractor/In-House Publication)

1 June 1999

FROM: PROI (TI) (STINFO)

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-TP-FY99-0110**
   Fajardo and Tam, "High Resolution Infrared Absorption Spectroscopy of Molecular Dopants in Cryogenic Solid
Parahydrogen"

Poster Session HEDM CONFERENCE

(Public Release)

Let me know which #'s are right. OK

see other page

High Resolution Infrared Absorption Spectroscopy of Molecular Dopants in Cryogenic Solid Parahydrogen

Mario E. Fajardo and Simon Tam

US Air Force Research Laboratory, Propulsion Directorate

(AFRL/PRSP Bldg. 8451, Edwards AFB, CA 93524-7680) mario_fajardo@ple.af.mil

Premature claims of successful energy storage in cryogenic solids date back to the National Bureau of Standards' Free Radicals program. Such errors typically result from reliance on unsupplemented calorimetric data, which shed little light on the mechanism of energy storage, *i.e.* chemical identities of the energetic species and microscopic structures within the trapping medium. **Only spectroscopic measurements provide the species and structure specific information required for directed incremental progress towards higher stored energy densities.**

In HEDM program funded studies, Oka and co-workers pioneered the use of high resolution spectroscopic techniques in solid parahydrogen (pH_2). Our rapid vapor deposition sample preparation technique now enables us to trap virtually any volatilizable species in solid pH_2. We present results of high resolution infrared absorption experiments on pH_2 solids doped with isolated molecules and small clusters.

13 PPM CH_4/pH_2 d≈3mm
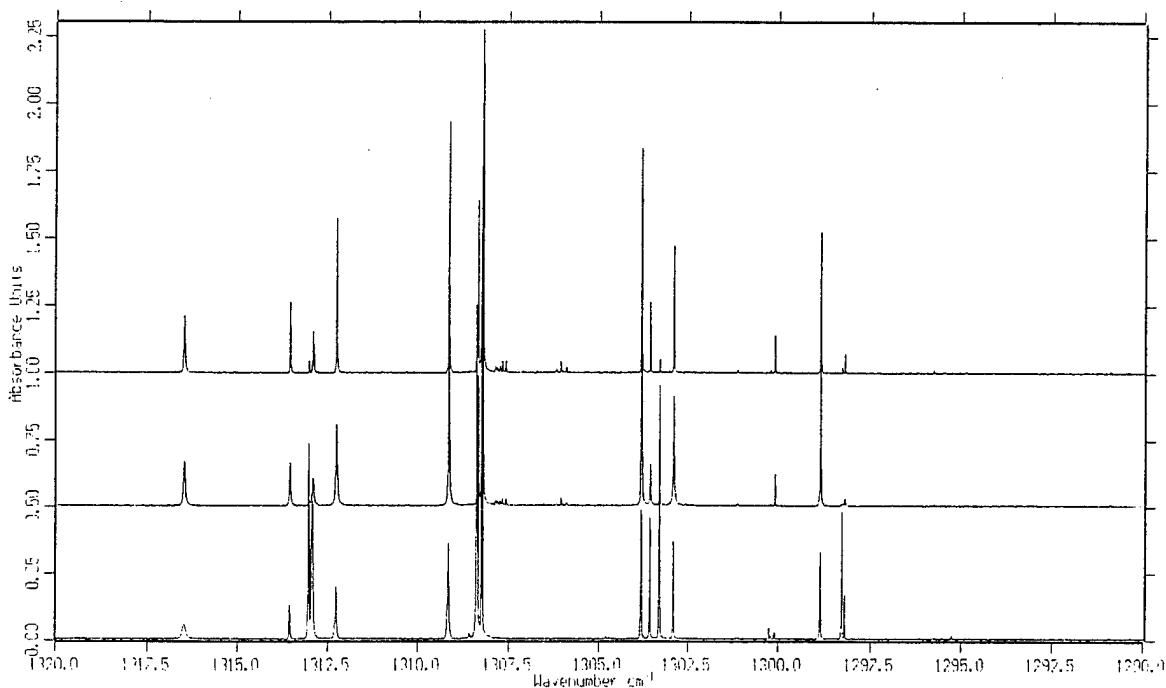
st27011.8   annealed   T=2.4K
st27011.4   annealing   T=4.8K
st27011.2   as deposited T=2.4K   resolution = 0.0075 cm⁻¹

OBJECTIVE

Develop infrared (IR) absorption spectroscopic diagnostics for HEDM doped cryogenic parahydrogen (pH_2) solids.

APPROACH

Collect high resolution IR spectra of pH_2 solids doped with <u>non-energetic</u> species: prototypical diatomic, triatomic, linear polyatomic, symmetric top, and spherical top dopant molecules.

Model data as "matrix-perturbed" gas phase spectra, if possible. Develop new spectroscopic models in collaboration with AFRL/Edwards Theory group, as necessary.

SUMMARY

Many, but not all, molecular dopants exhibit very sharp (~0.01 cm^{-1} FWHM) IR absorption lines in solid pH_2, providing an extremely detailed window into trapping site structures and dynamics.

Model for spherical top molecules trapped in single substitutional sites in fcc and hcp solid pH_2 developed in collaboration with Prof. T. Momose of Kyoto U. is completely successful in explaining spectra of CH_4/pH_2 system. Model of trapped diatomic molecules forthcoming.

FUTURE DIRECTIONS

Develop model for dopants trapped in multi-substitutional vacancies.

Include effects of lattice relaxation via quantum Monte Carlo methods.

9 ~~PPM~~ *ppm* C₂H₂/pH₂ d≈3mm

$9 \text{ ppm } C_2H_2/pH_2 \quad d \approx 3mm$
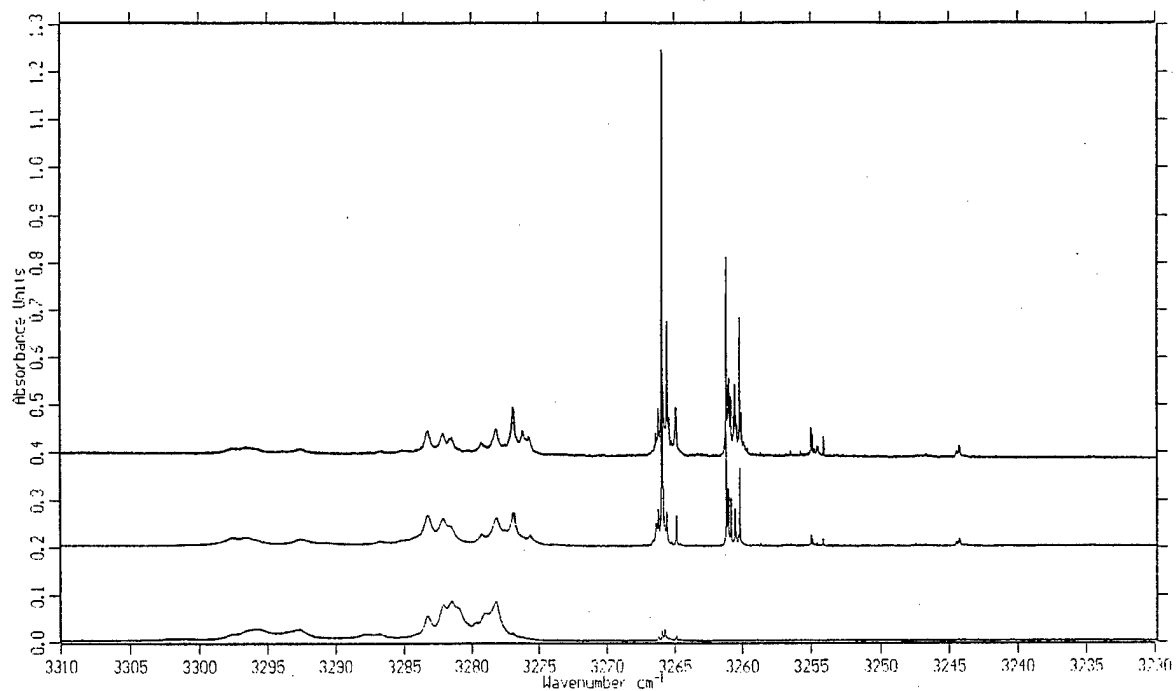
st28034.13   annealed   T=2.4K
st28034.7   annealing   T=4.8K
st28034.5   as deposited T=2.4K   resolution = 0.005 cm⁻¹

ST28004.5

13 ~~PPM~~ *ppm* CO/pH₂ d≈3mm

$13 \text{ ppm } CO/pH_2 \quad d \approx 3mm$
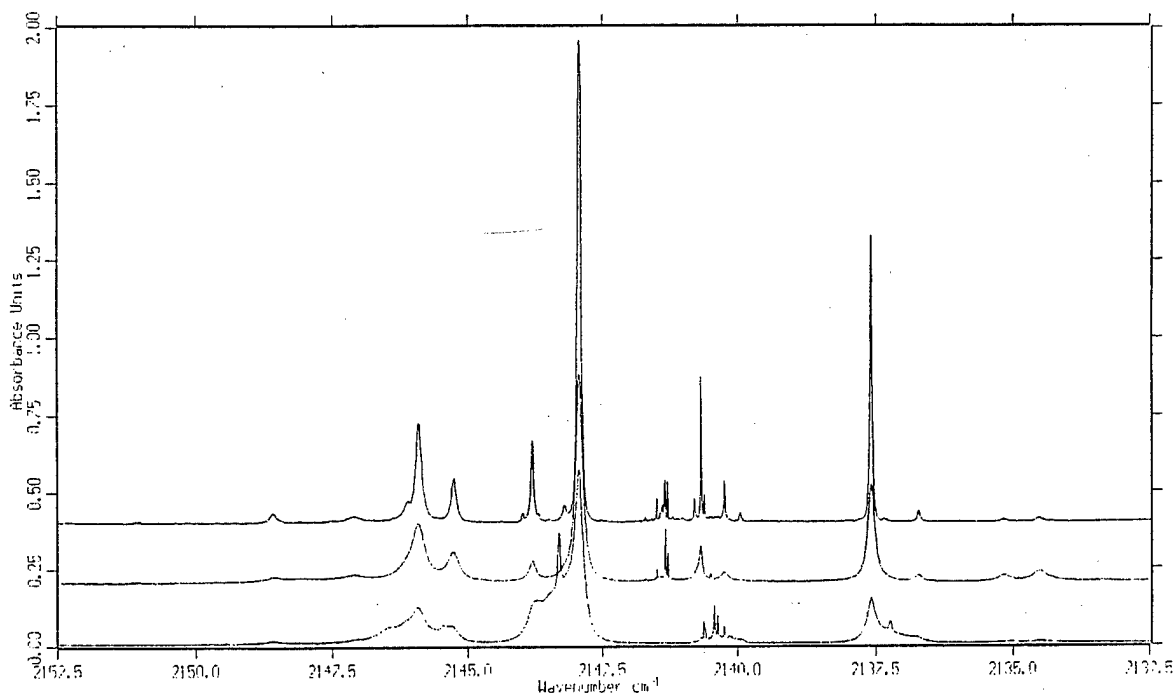
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st27017.14   annealing   T=4.8K
st27017.10   as deposited T=2.4K   resolution = 0.0075 cm⁻¹

ST27017.10

$^{13}C^{16}O/pH_2$ d≈3mm
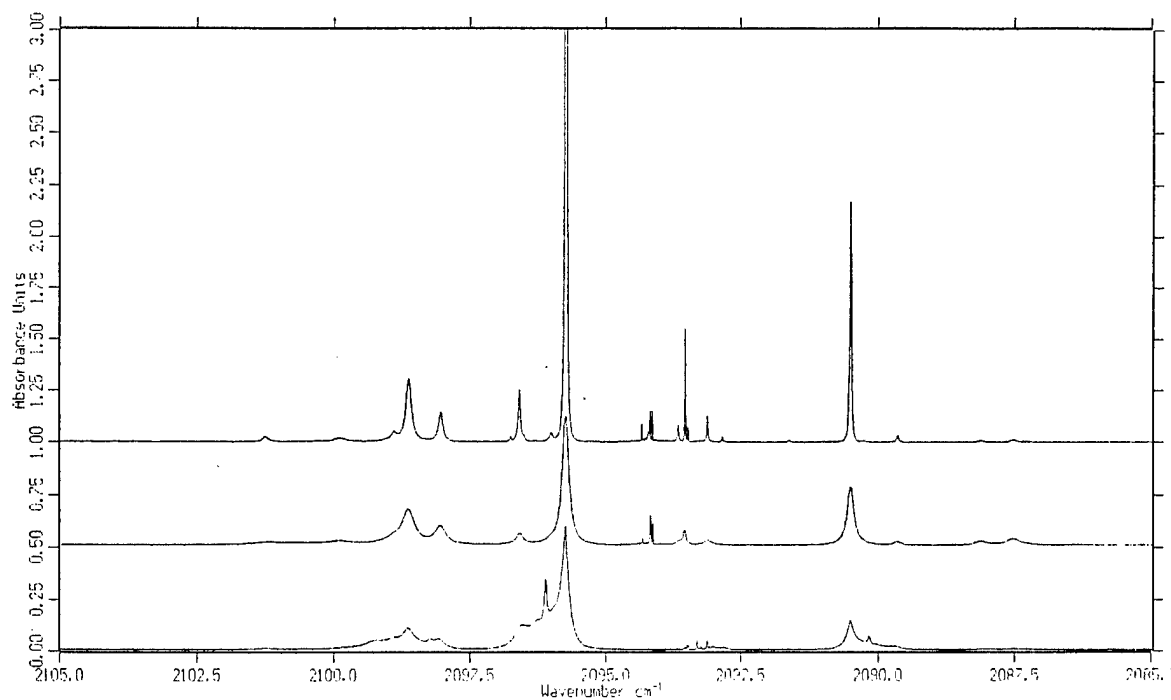
st28082.6   annealed   T=2.4K
st28082.4   annealing   T=4.8K
st28082.2   as deposited T=2.4K   11 PPM $^{13}CO/pH_2$ resolution = 0.005 cm⁻¹

$^{13}C^{18}O/pH_2$ d≈3mm
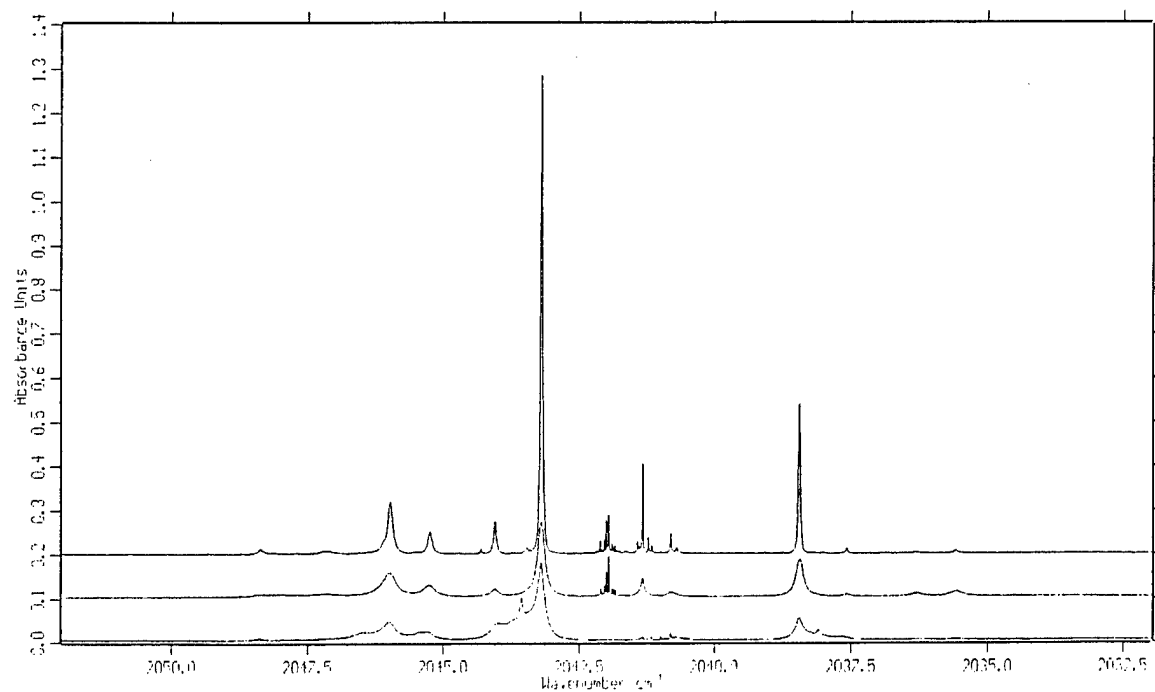
st28085.5   annealed   T=2.4K
st28085.3   annealing   T=4.8K
st28085.1   as deposited T=2.4K   29 PPM $^{13}CO/pH_2$ resolution = 0.005 cm⁻¹

90 ~~PPM~~ *PPM* $H^{35}Cl/pH_2$ d≈3mm

Absorbance Units
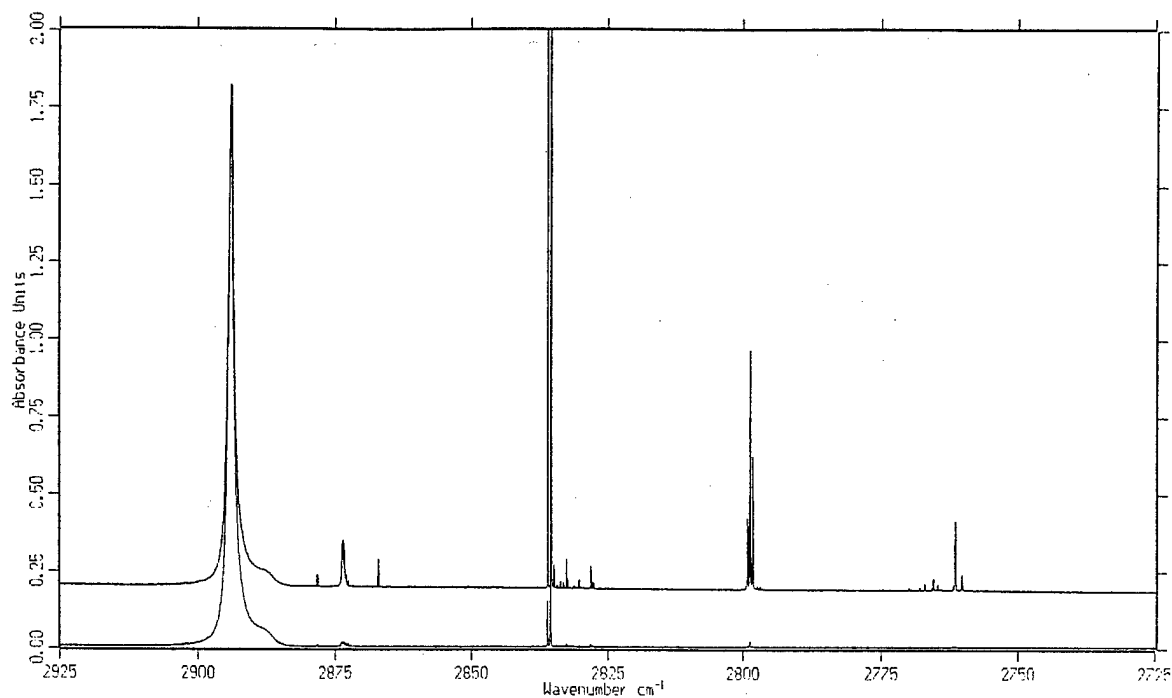
st27079.11 annealed   T=2.4K
st27079.7   as deposited T=2.4K
resolution = 0.005 cm⁻¹

ST27079.7

88 ~~PPM~~ *PPM* HCl/pH_2 d≈3mm

Absorbance Units

Wavenumber cm⁻¹
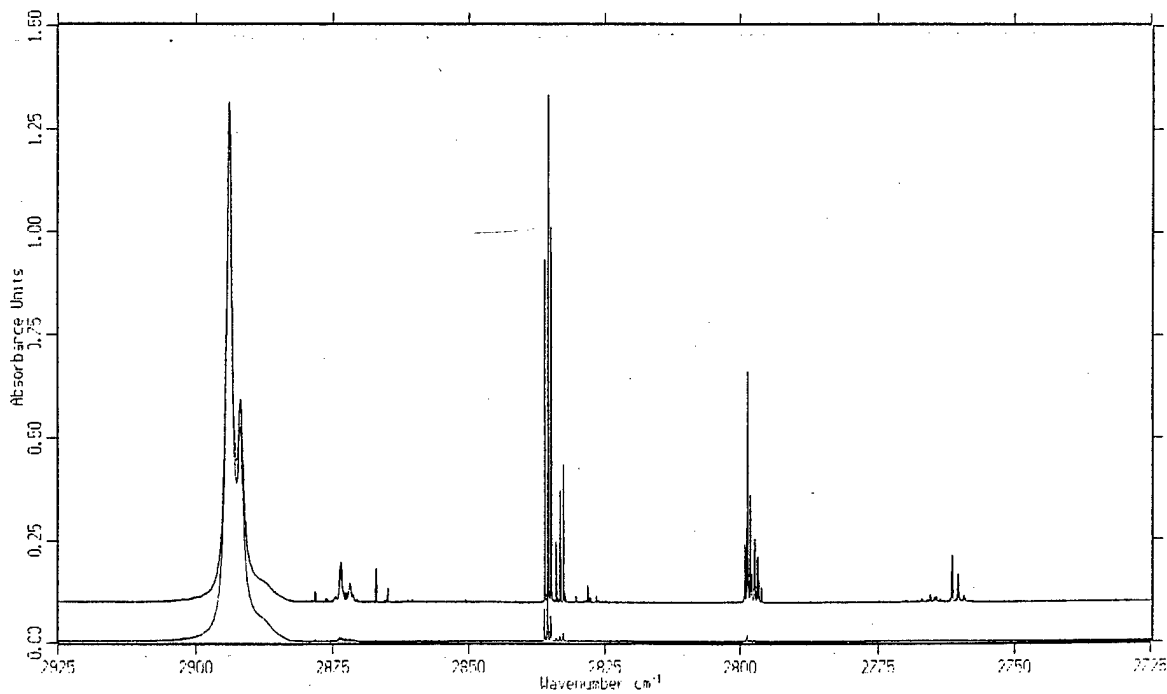
st27061.11 annealed   T=2.4K
st27061.7   as deposited T=2.4K
resolution = 0.0075 cm⁻¹

94 PPM H^{37}Cl/pH$_2$ d≈3mm
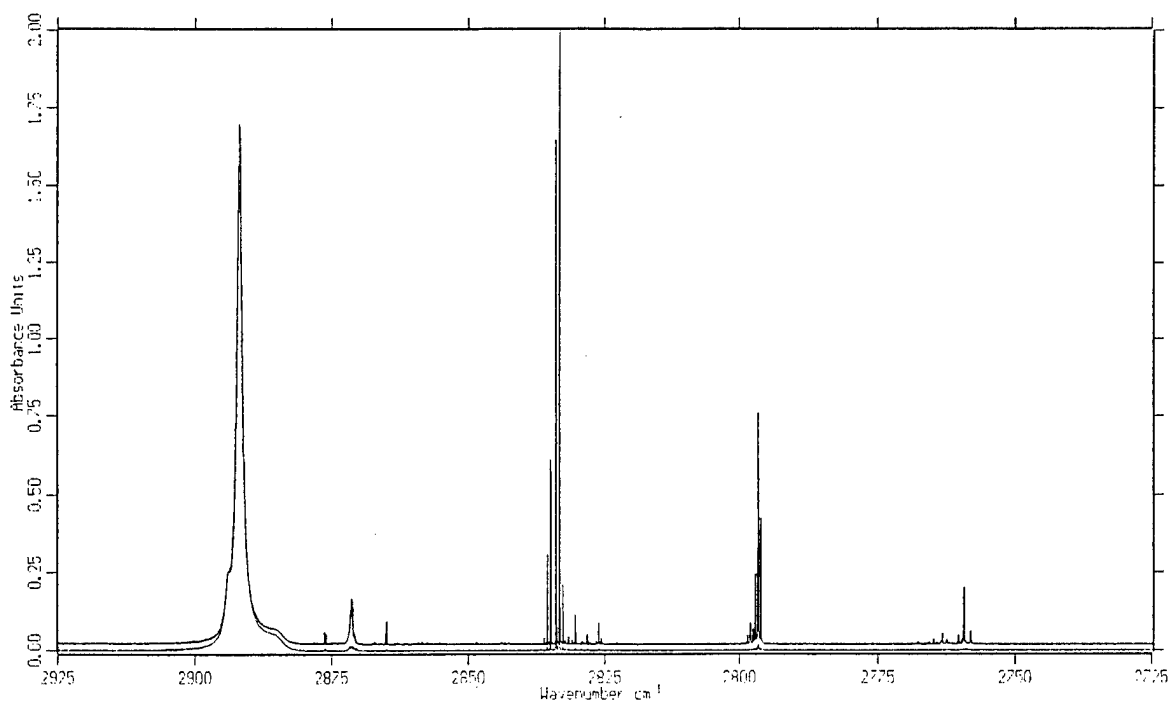
st27103.6   annealed   T=2.4K
st27103.2   as deposited T=2.4K
resolution = 0.005 cm^{-1}

irreversible T dependences
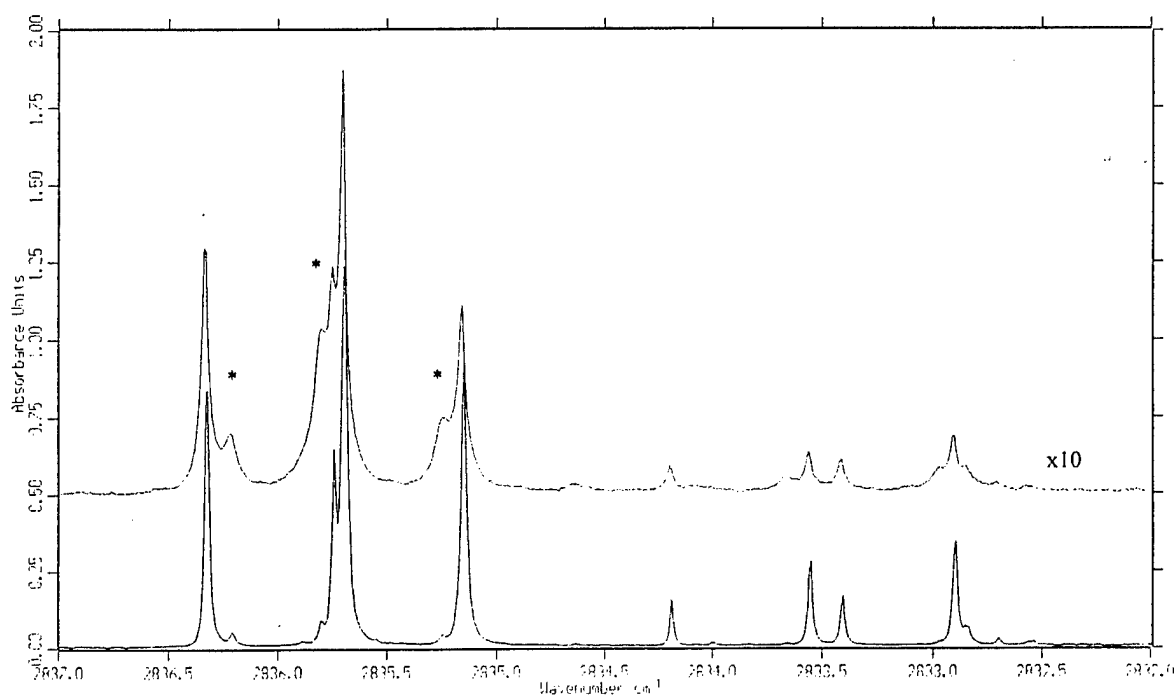
88 PPM HCl/pH$_2$ d≈3mm
st27061.7   as deposited T=2.4K
st27061.11 annealed   T=2.4K

reversible T dependences
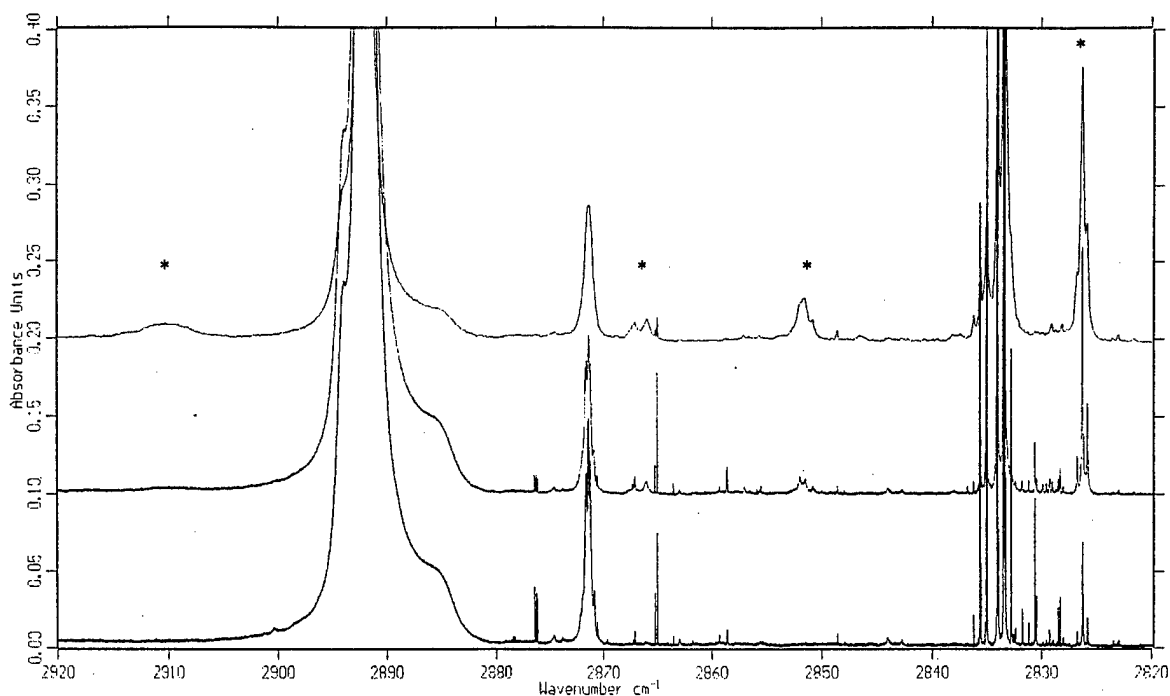
st27103.13 evaporating T≈10K   94 PPM $H^{37}Cl$
st27103.4   annealing   T=4.8K
st27061.11 annealed   T=2.4K

ST27103.4

gas phase HCl and (HCl)$_2$ transitions

R(1)   R(0)   "Q(0)"   P(1)

$v_1^+ \perp$ $v_1^+ \perp$ $v_2^+ \parallel$ $v_2^+ \parallel$
K=1←0   K=0←0   K=1←0   K=0←0

BS $v_1^+ \perp$ BS $v_2^+ \parallel$
K=1←0   K=0←0

                  $v_1^- \perp$ $v_1^- \perp$ $v_2^- \parallel$
                  K=1←0   K=0←0   K=0←0

simulated absorbance (arb.)

wavenumber (cm^{-1})

$(HCl)_2$ ν_2^+ region

st27061.11	annealed	T=2.4K	88 PPM HCl
st27097.6	annealed	T=2.4K	33 PPM H^{37}Cl
st27073.17	annealed	T=2.4K	30 PPM H^{35}Cl

$(HCl)_3$

st27061.11	annealed	T=2.4K	88 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM H^{37}Cl
st27079.11	annealed	T=2.4K	90 PPM H^{35}Cl

$(HCl)_4$
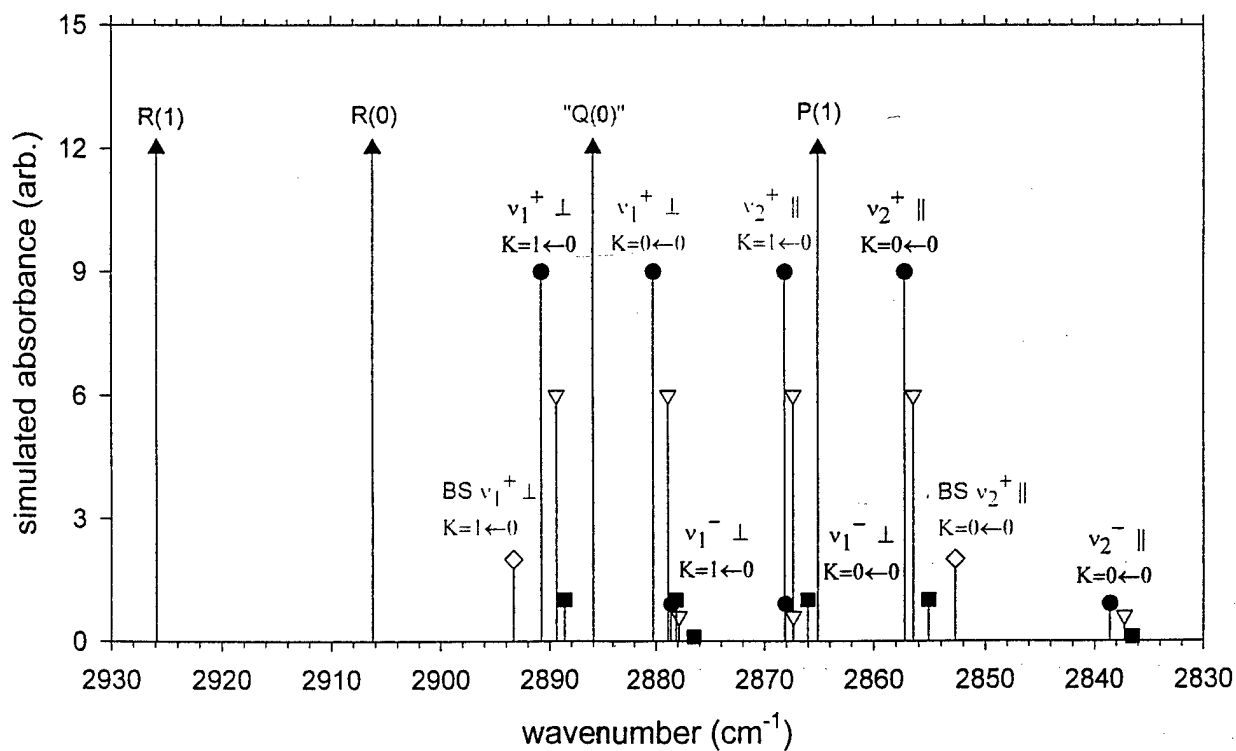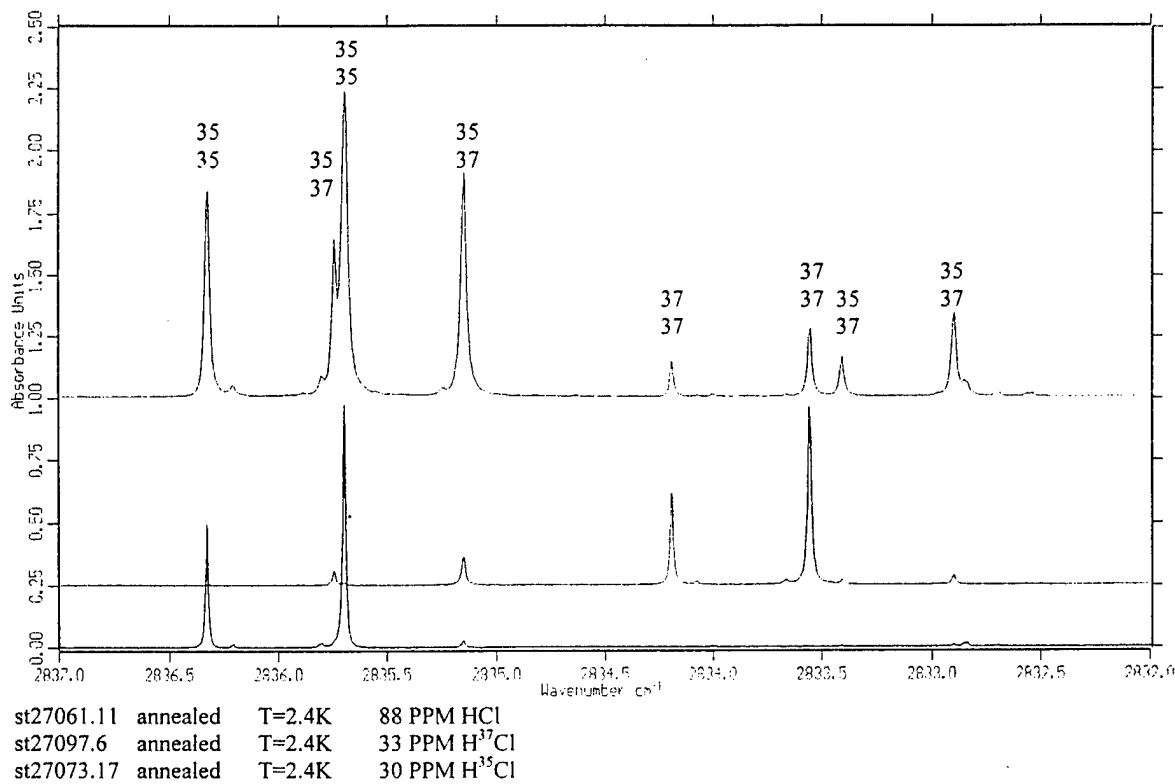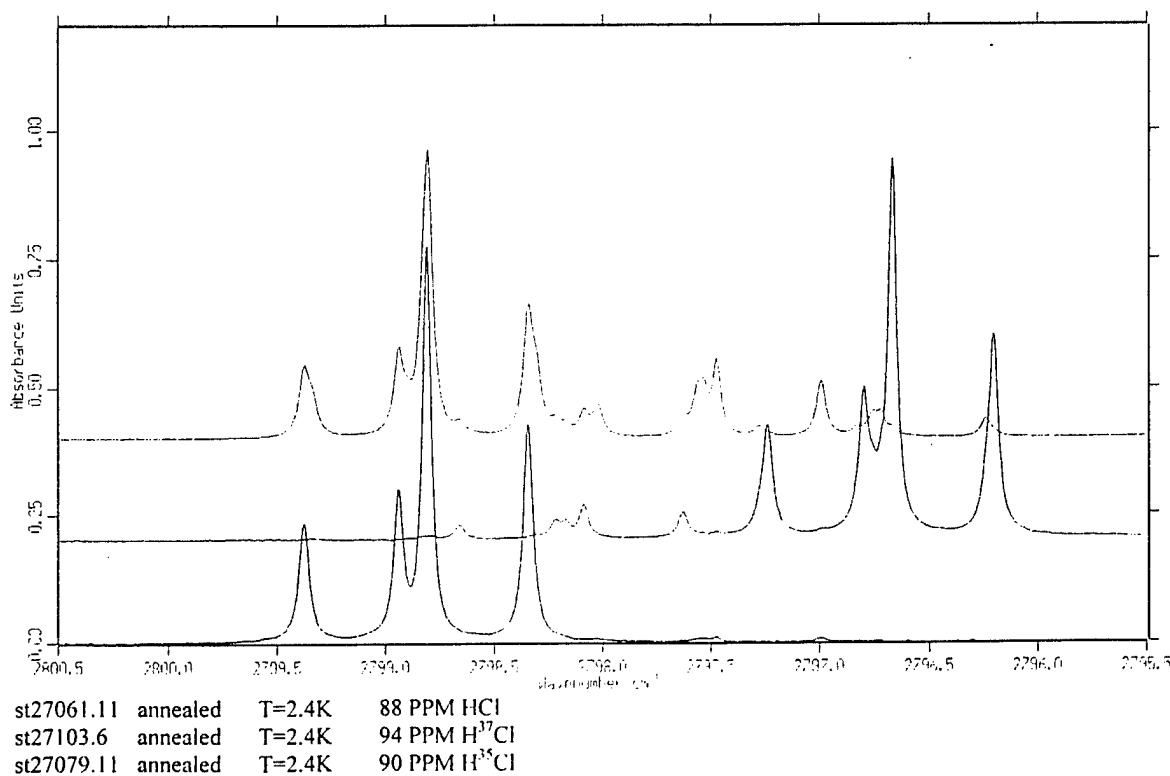
ST27103.6

st27067.10   annealed   T=2.4K   494 PPM HCl
st27103.6   annealed   T=2.4K   94 PPM H^{37}Cl
st27085.9   annealed   T=2.4K   284 PPM H^{35}Cl

123 ~~PPM~~ *ppm* HF/pH$_2$ d≈3mm
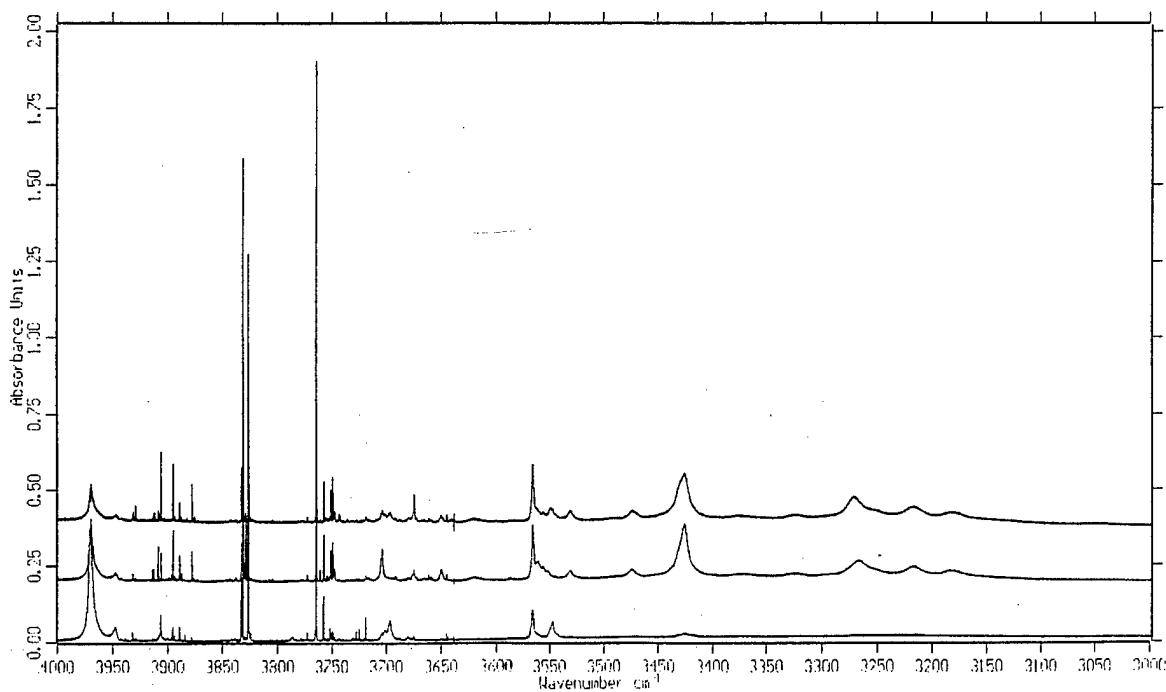
st27115.15   annealed   T=2.4K
st27115.13   annealing   T=4.8K
st271215.9   as deposited T=2.4K   resolution = 0.005 cm^{-1}

(HF)n/pH2
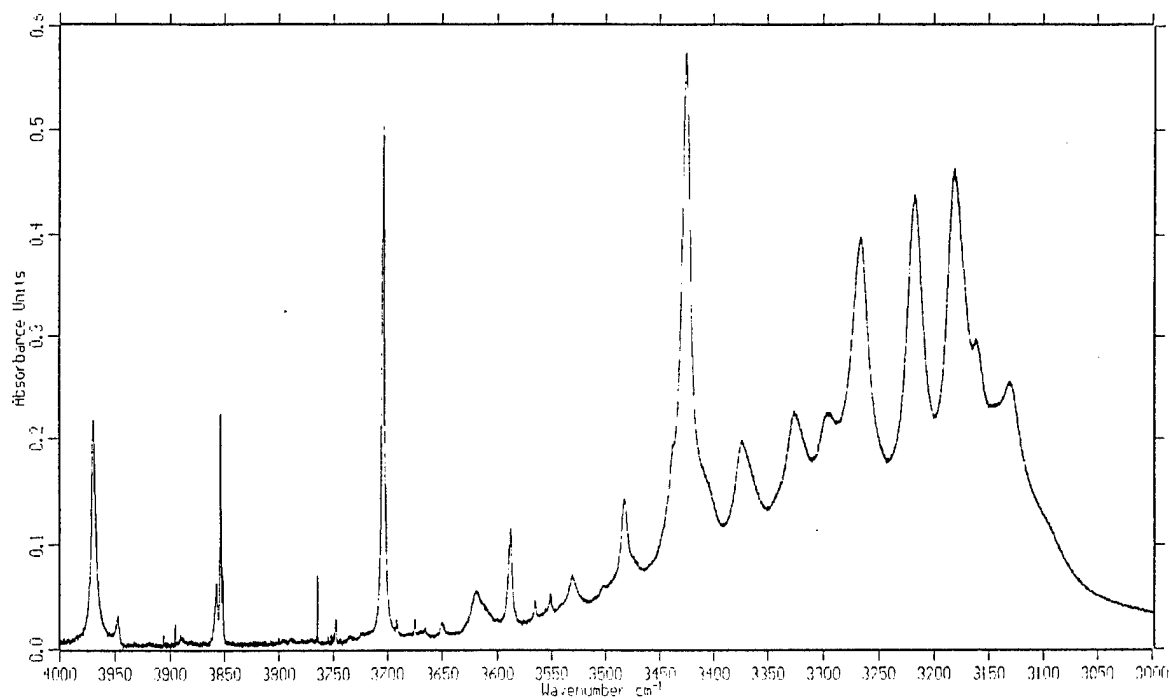
st27133.15   sample burnoff   T~10K   268 PPM HF/pH2   resolution = 0.1 cm⁻¹

HF-HCl/pH2

st27115.15   annealed   T=2.4K
st27115.13   annealing   T=4.8K
st27115.9   as deposited T=2.4K   123 PPM HF/pH2 d≈3mm   resolution = 0.005 cm⁻¹

260 PPM HBr/pH$_2$ d≈3mm

Absorbance Units — Wavenumber cm^{-1} (2600 to 2400)
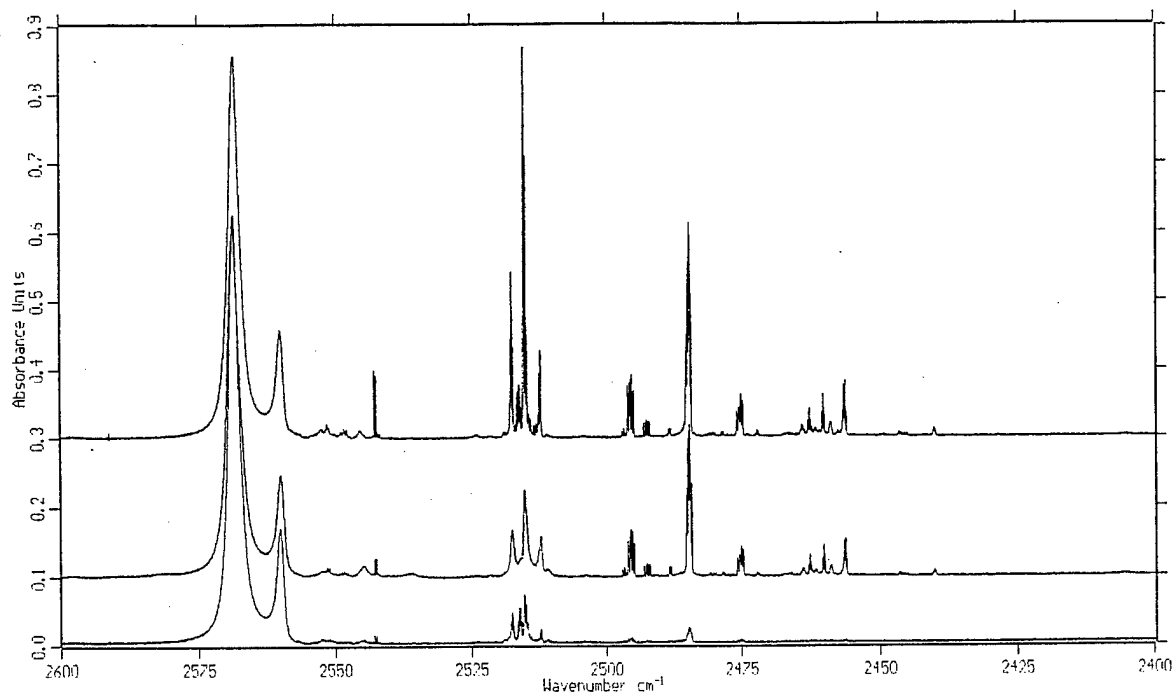
st27145.9   annealed   T=2.4K
st27145.7   annealing   T=4.8K
st27145.5   as deposited T=2.4K   resolution = 0.005 cm^{-1}

ST27145.5

(HBr)$_2$/pH$_2$
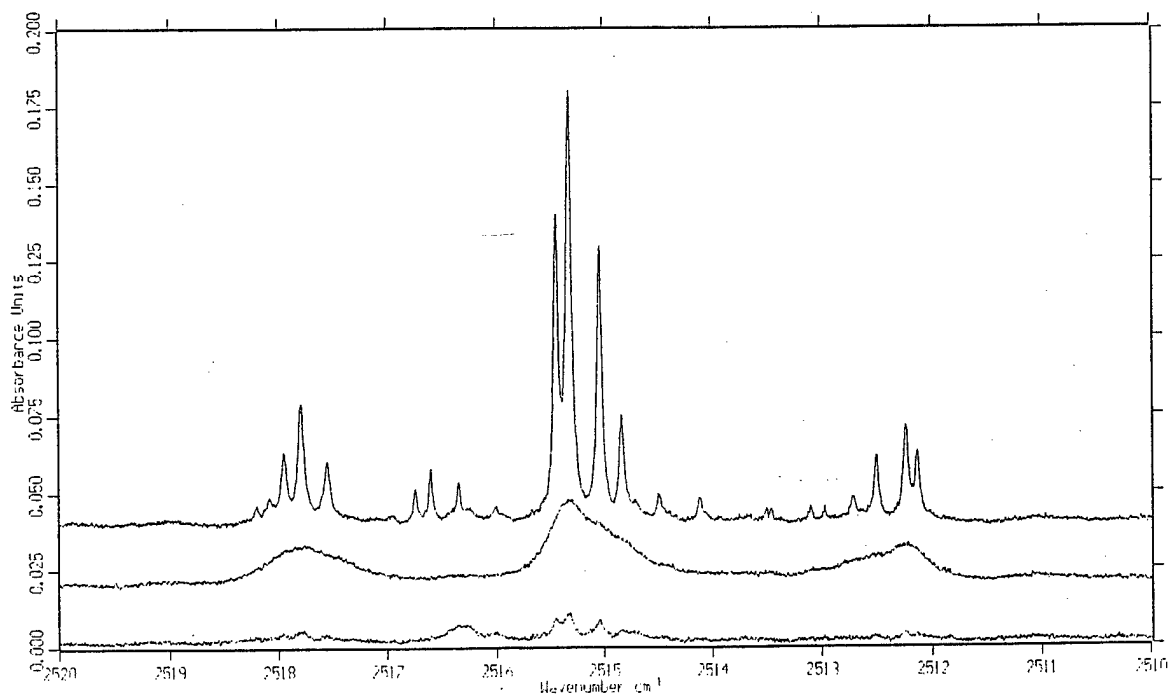
Absorbance Units — Wavenumber cm^{-1} (2520 to 2510)

st27140.9   annealed   T=2.4K
st27140.7   annealing   T=4.8K
st27140.5   as deposited T=2.4K   80 PPM HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

HCl-(HF, HCl, HBr)/pH$_2$

st27145.9   annealed   T=2.4K
st27145.7   annealing   T=4.8K
st27145.5   as deposited T=2.4K   260 PPM HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

2.4 PPM CH$_3$F/pH$_2$ d≈3mm

st28060.15   annealed   T=2.4K
st28060.11   annealing   T=4.8K
st28060.6+7   as deposited T=2.4K   resolution = 0.005 cm^{-1}

^{1}H Spin Relaxation in CH$_3$F/pH$_2$
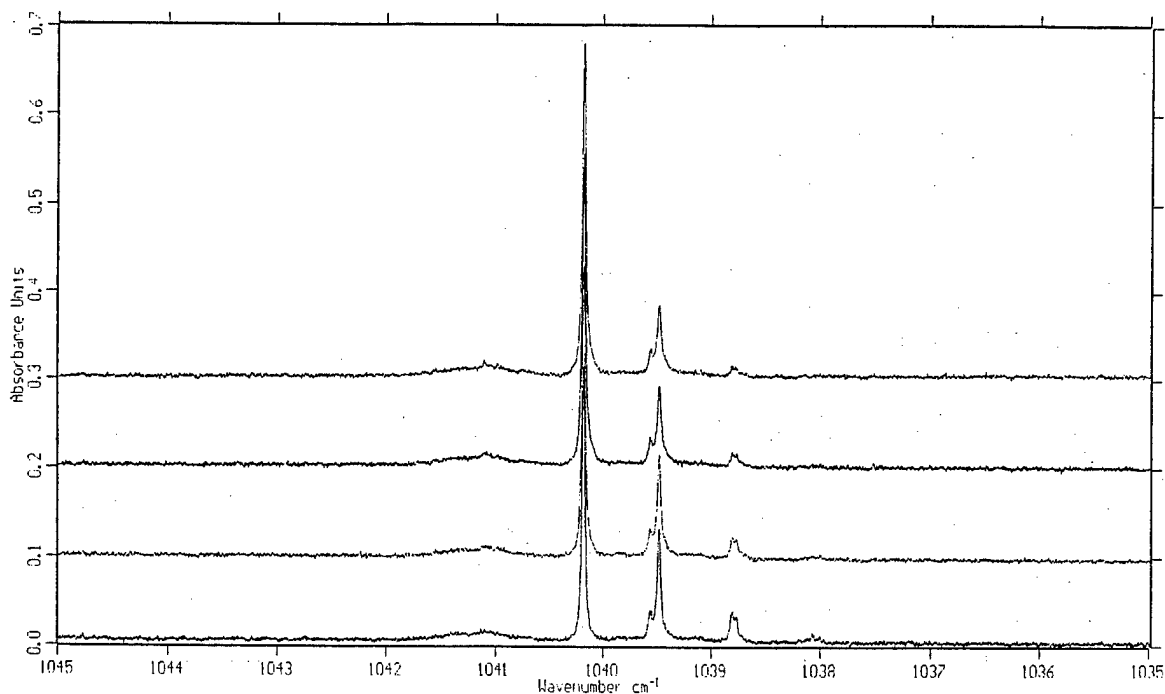
st28060.7	after 100 min	T=2.4K	st28060.3	after 30 min	T=2.4K	
st28060.6	after 70 min	T=2.4K	st28060.2	as deposited	T=2.4K	resolution = 0.005 cm^{-1}

ST28060.2

(CH$_3$F)$_2$/pH$_2$
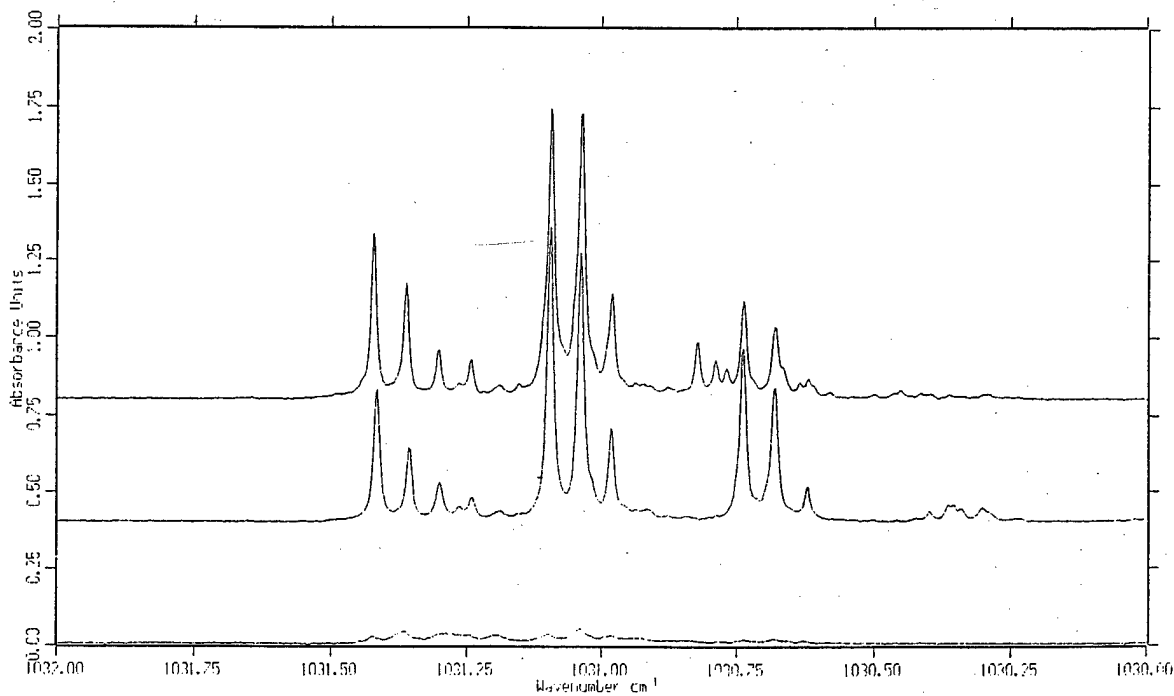
st28044.11	annealed	T=2.4K
st28044.7	annealing	T=4.8K
st28044.3	as deposited	T=2.4K

30 PPM CH$_3$F/pH$_2$ resolution = 0.005 cm^{-1}

ST28044.1

SUPPLEMENTAL MATERIALS

for the poster:

High Resolution Infrared Absorption Spectroscopy of Molecular Dopants in Cryogenic Solid Parahydrogen

Mario E. Fajardo and Simon Tam
US Air Force Research Laboratory, Propulsion Directorate
(AFRL/PRSP Bldg. 8451, Edwards AFB, CA 93524-7680) mario_fajardo@ple.af.mil

Consisting of spectra of NON-ENERGETIC species trapped in solid hydrogen at low concentrations. These data encompass prototypical diatomic (CO, HCl, HF, HBr), triatomic (CO_2, N_2O, H_2O), linear polyatomic (C_2H_2), symmetric top (NH_3, CH_3F), and spherical top (CH_4) molecular dopants. The basic research activity of understanding these spectra will aid in the future characterization of HEDM cryosolid propellants.
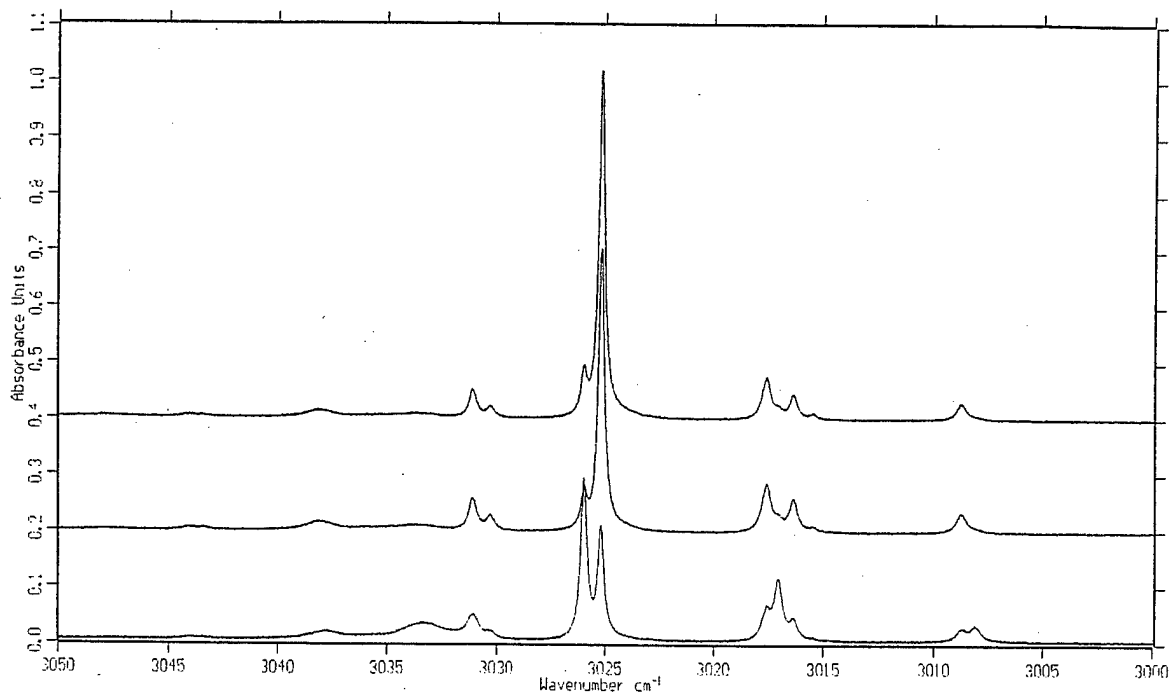
13 PPM CH₄/pH₂ d≈3mm

st27011.8	annealed	T=2.4K
st27011.4	annealing	T=4.8K
st27011.2	as deposited T=2.4K	resolution = 0.0075 cm⁻¹

ST27011.2
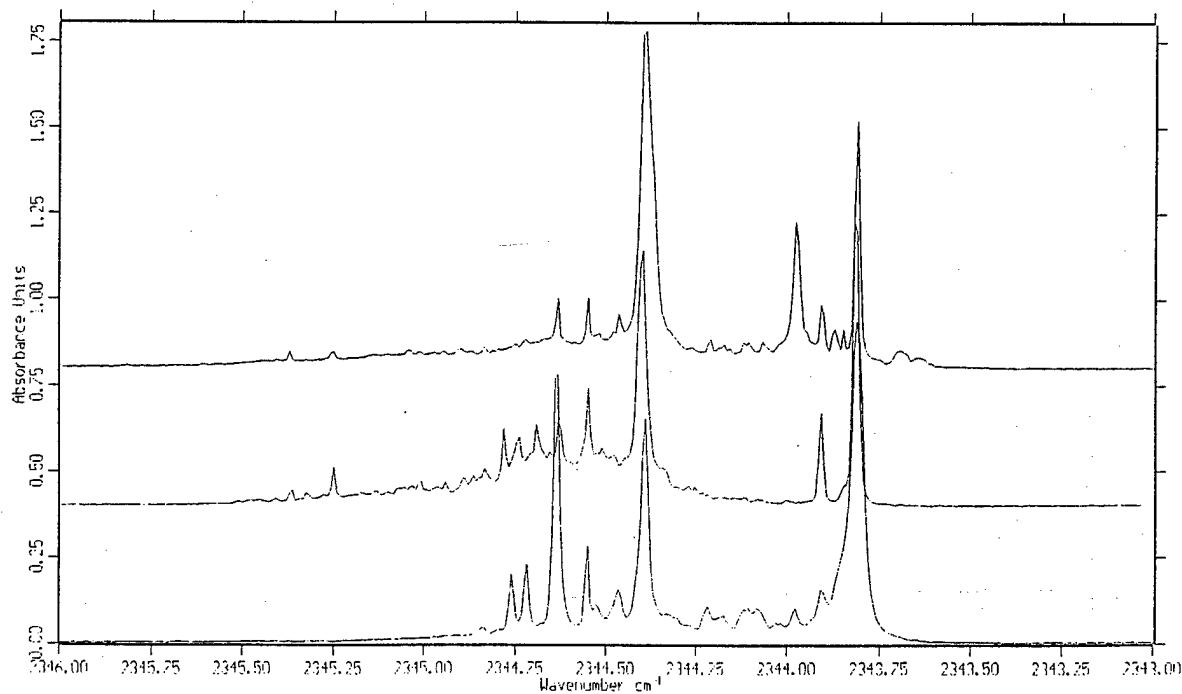
1 PPM CO₂/pH₂ d≈3mm

st27025.11	annealed	T=2.4K
st27025.9	annealing	T=4.8K
st27025.7	as deposited T=2.4K	resolution = 0.005 cm⁻¹

1 ~~PPM~~ ppm N_2O/pH_2 d≈3mm
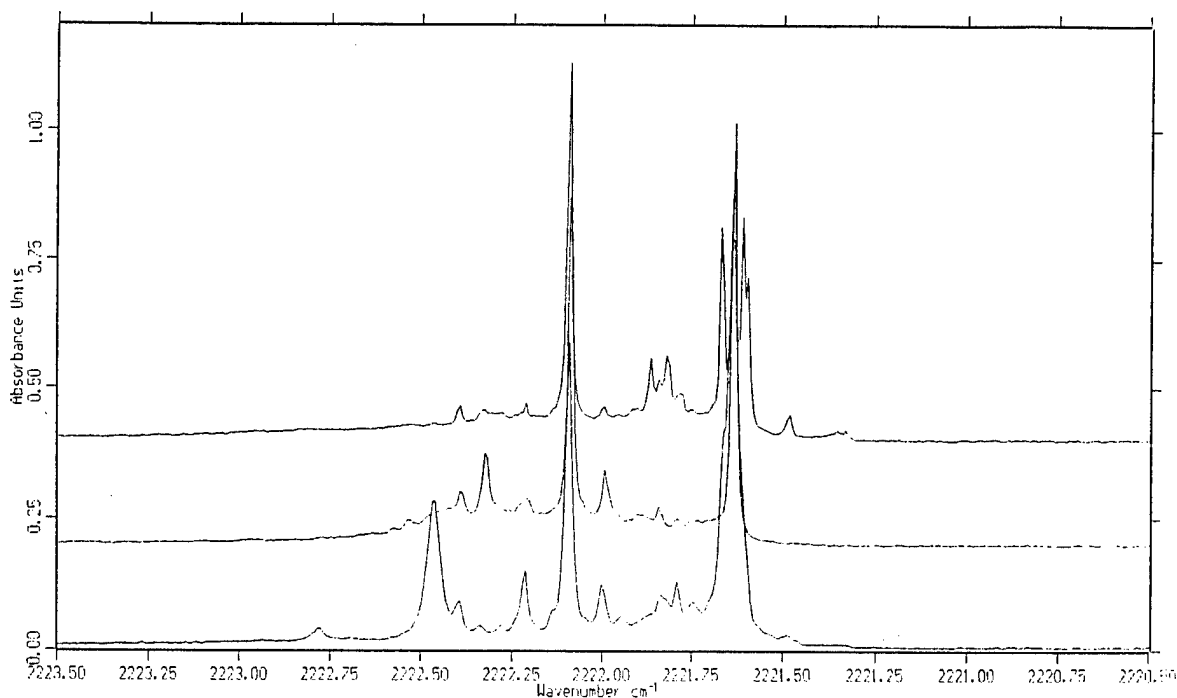
st2702~~5~~.14   annealed   T=2.4K
st2702~~5~~.12   annealing   T=4.8K
st2702~~5~~.6   as deposited T=2.4K   resolution = 0.005 cm^{-1}
31

ST27031.c

4 ~~PPM~~ ppm NH_3/pH_2 d≈3mm
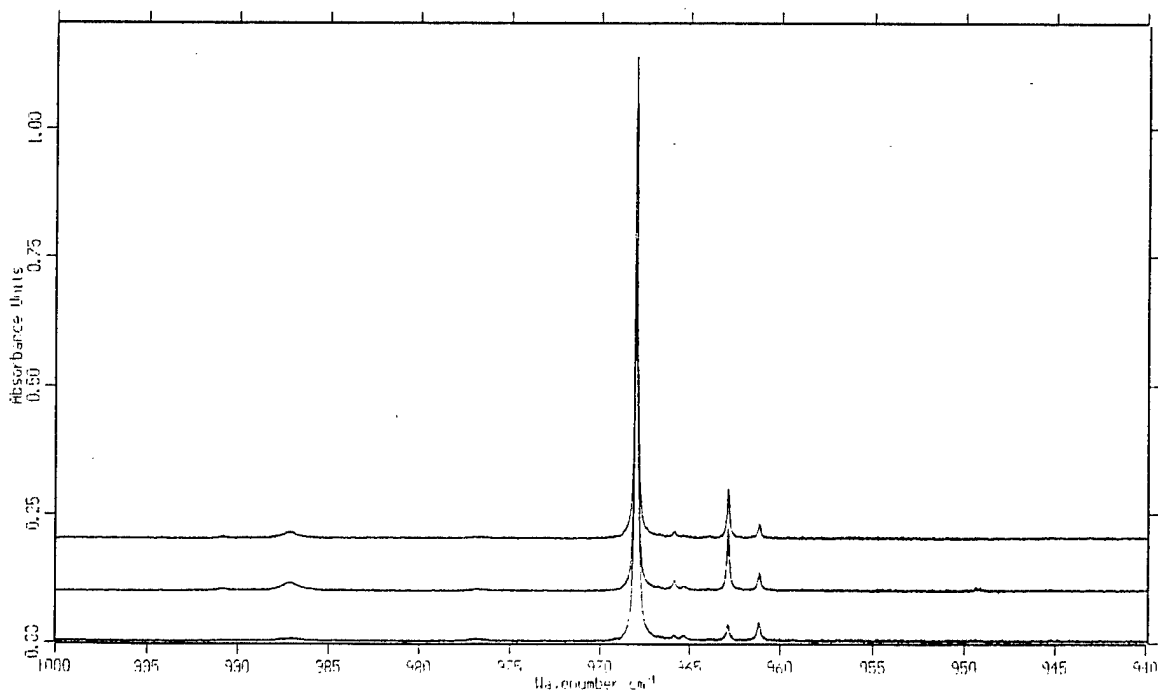
st27036.12   annealed   T=2.4K
st27036.10   annealing   T=4.8K
st27036.8   as deposited T=2.4K .   resolution = 0.005 cm^{-1}

4 PPM NH₃/pH₂ d≈3mm

$$\text{4 } ^{ppm}\text{PPM NH}_3/\text{pH}_2 \quad d \approx 3\text{mm}$$
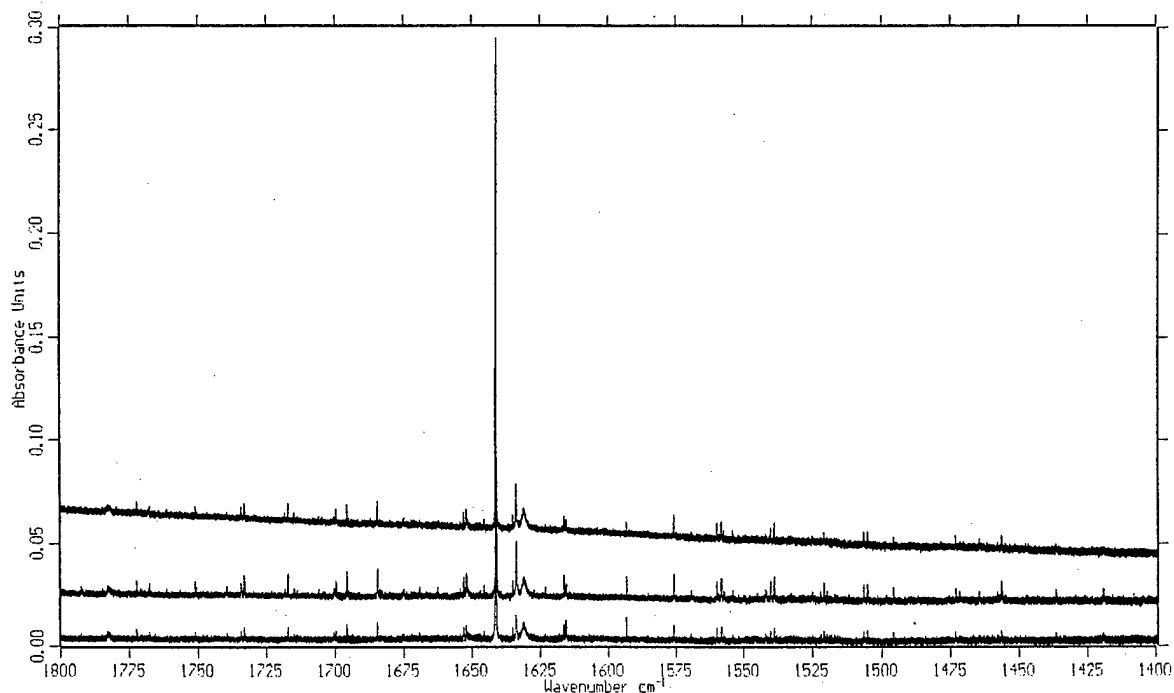
st27036.12   annealed   T=2.4K
st27036.10   annealing   T=4.8K
st27036.8   as deposited T=2.4K   resolution = 0.005 cm⁻¹

ST27036.8

$$\text{8 } ^{ppm}\text{PPM HCl/pH}_2 \quad d \approx 3\text{mm}$$

st27055.11   annealed   T=2.4K
st27055.4   as deposited T=2.4K
resolution = 0.05 cm⁻¹

reversible T dependences
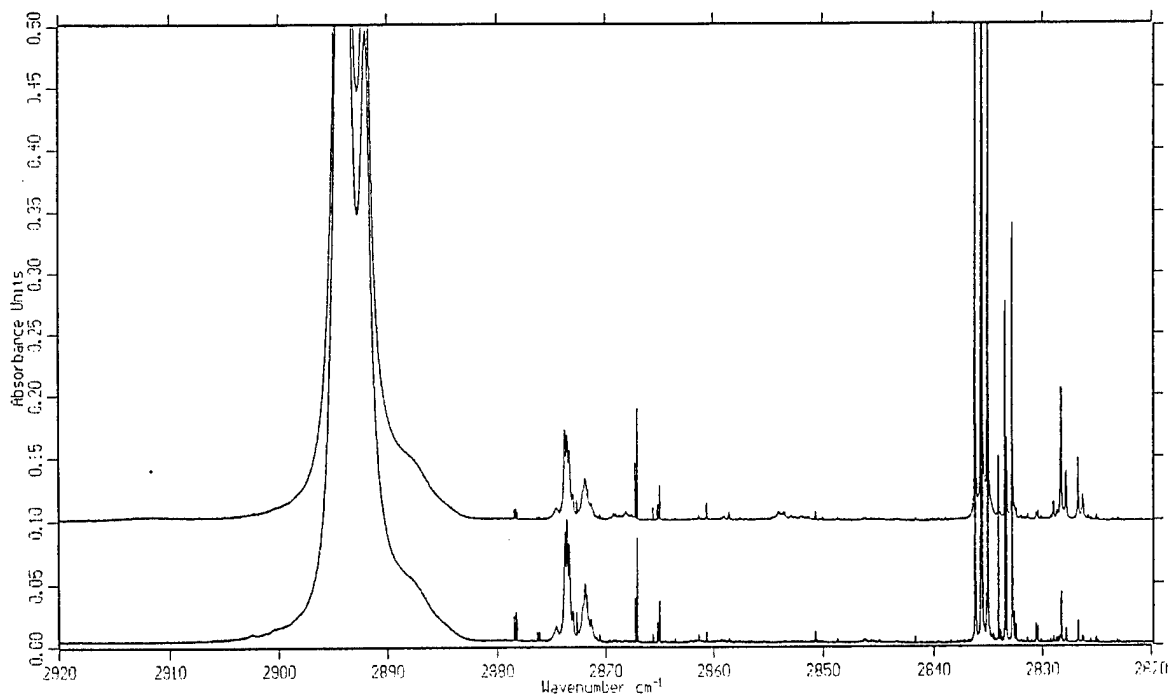
88 PPM HCl
st27061.9   annealing   T=4.8K
st27061.11 annealed   T=2.4K

ST27061.9

$(HCl)_2$ v_2^+ region
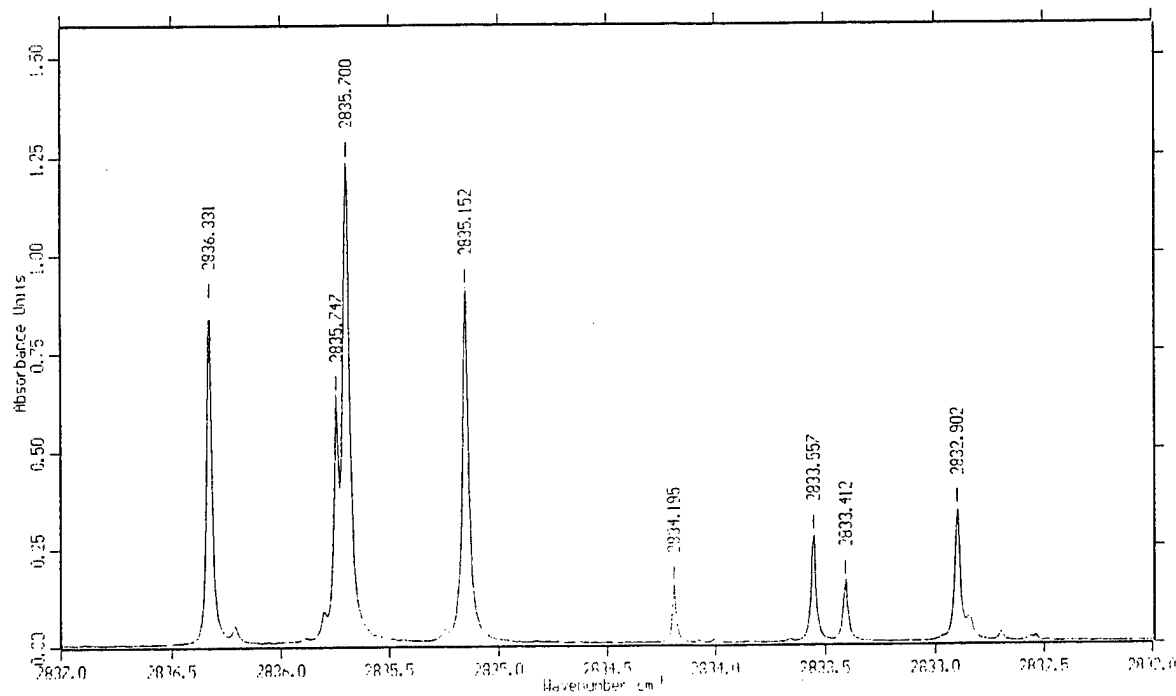
st27061.11   annealed   T=2.4K   88 PPM HCl

494 ~~PPM~~ ppm HCl/pH$_2$ d≈3mm
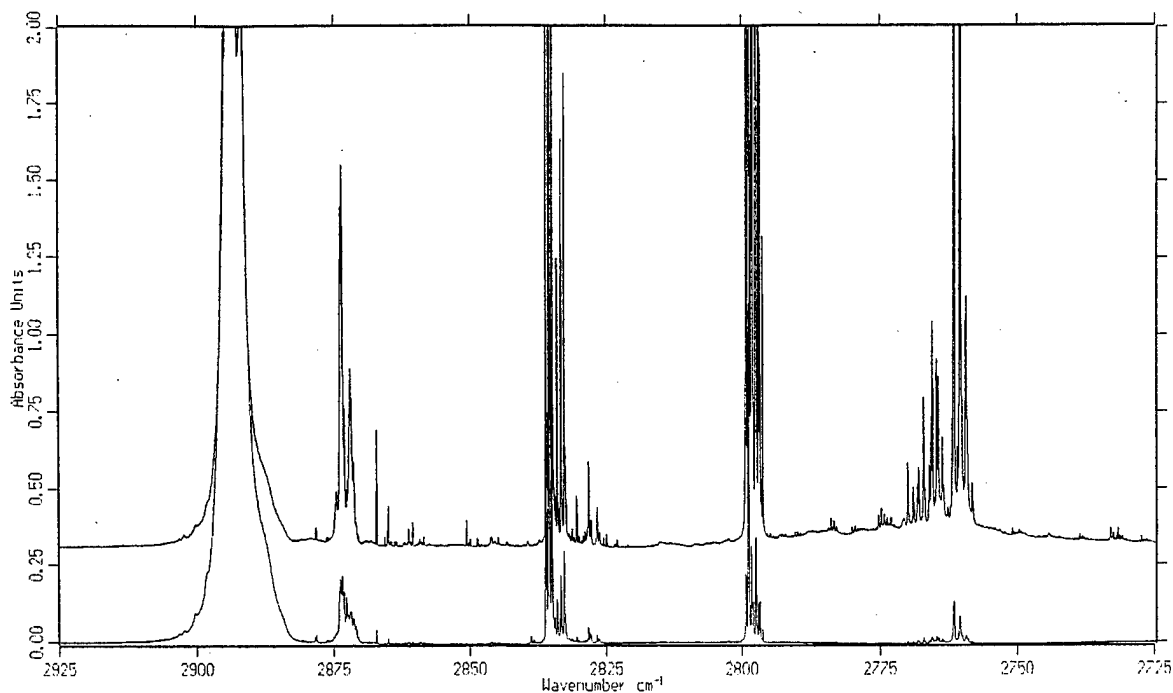
st27067.10 annealed   T=2.4K
st27067.6   as deposited T=2.4K
resolution = 0.0075 cm^{-1}

ST27067.6

30 ~~PPM~~ ppm H^{35}Cl/pH$_2$ d≈3mm
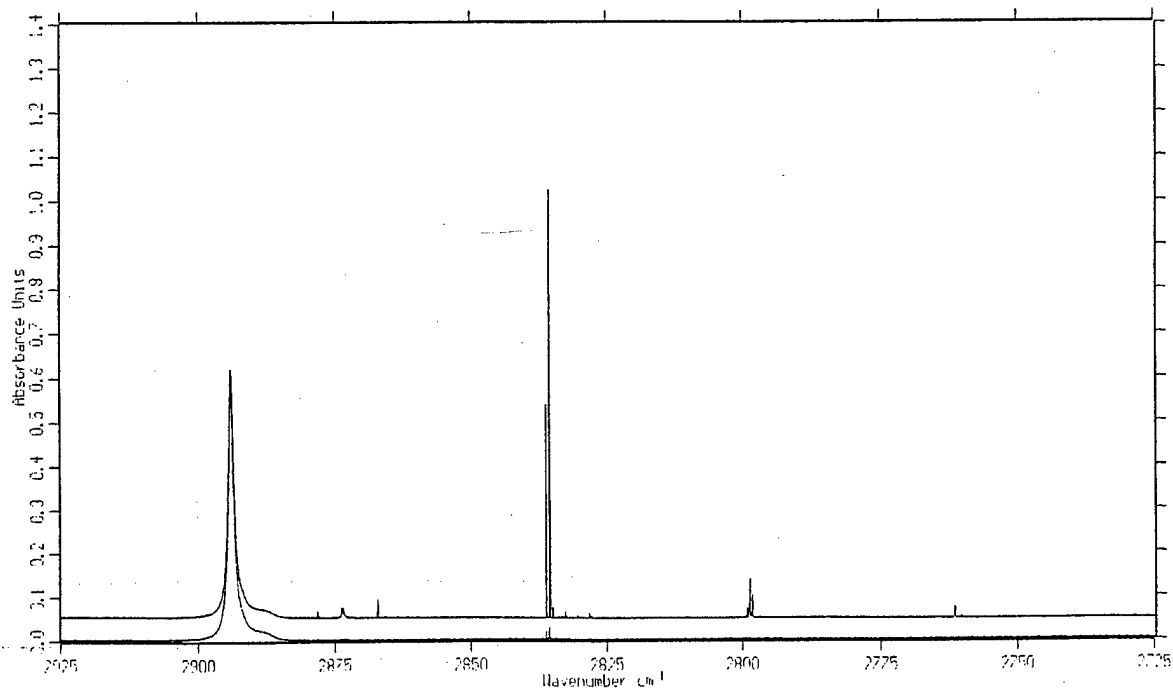
st27073.17 annealed   T=2.4K
st27073.9   as deposited T=2.4K
resolution = 0.005 cm^{-1}

reversible T dependences
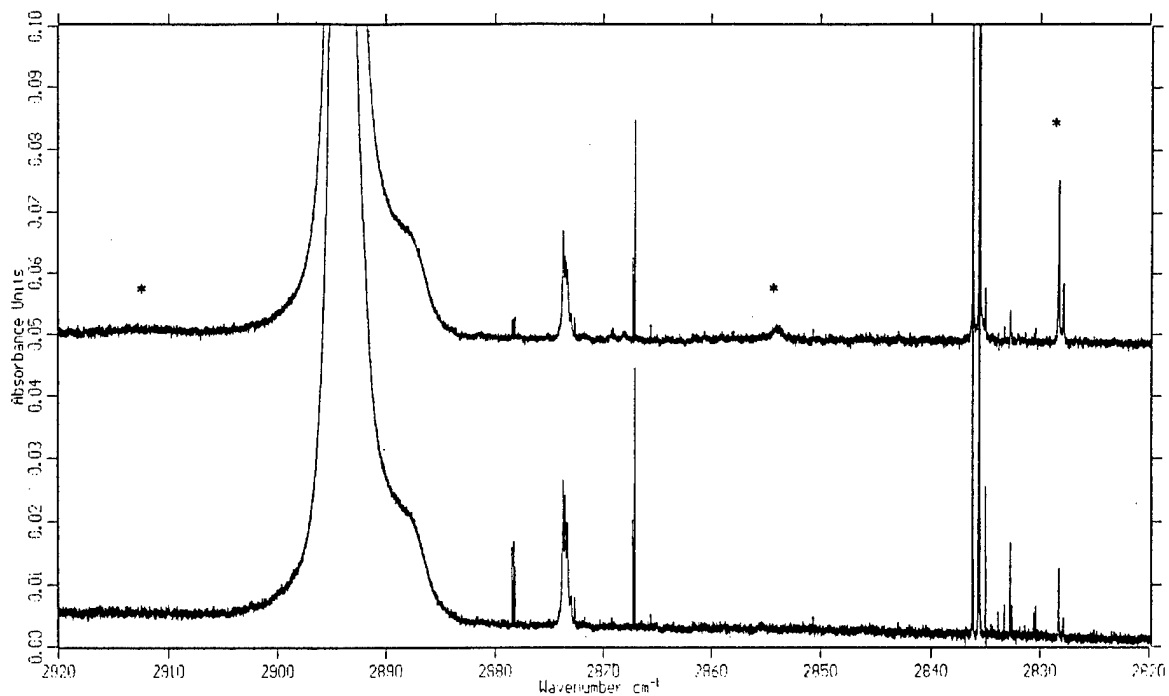
30 PPM H^{35}Cl
st27073.11 annealing   T=4.8K
st27073.17 annealed   T=2.4K

ST27073.11

284 PPM H^{35}Cl/pH$_2$ d≈3mm
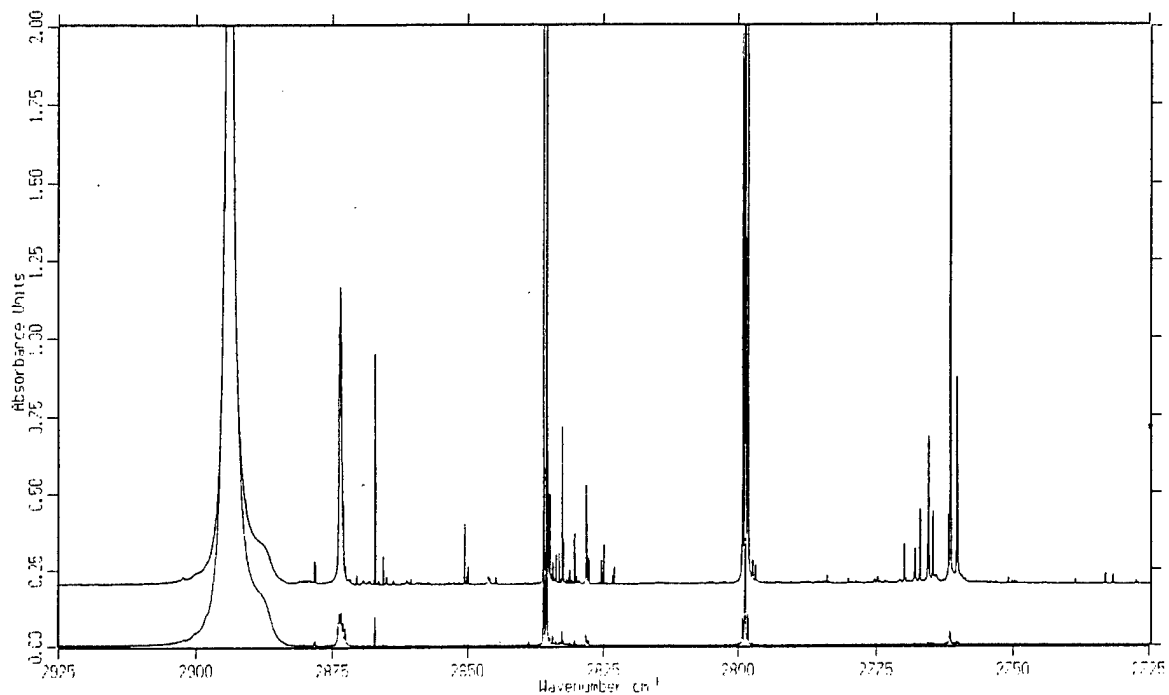
st27085.9   annealed   T=2.4K
st27085.5   as deposited T=2.4K
resolution = 0.005 cm^{-1}

33 ~~PPM~~ ppm H^{37}Cl/pH$_2$ d≈3mm
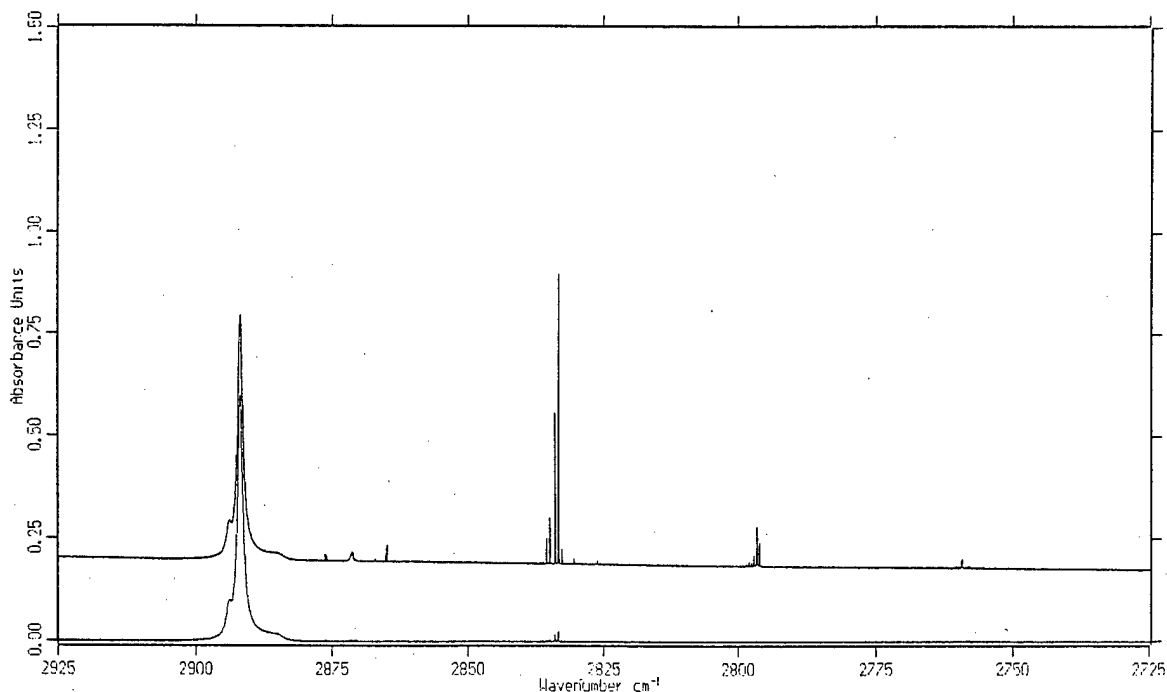
st27097.6   annealed   T=2.4K
st27097.2   as deposited T=2.4K
resolution = 0.005 cm^{-1}

ST27097.2

HCl monomer shifts

species	line/band	gas phase (cm^{-1})	solid pH$_2$	gas-matrix
H^{35}Cl	R(1)	2925.8961	2912	14
	R(0)	2906.2464	2894.2	12.1
	"Q(0)"	2885.67	2873.86	
			2873.67	12.0
			2873.46	
			2873.14	
	P(1)	2865.0977	2854.12	
			2853.58	11.5
			2852.95	
H^{37}Cl	R(1)	2923.7315	2910.2	13.5
	R(0)	2904.1104	2892.1	12.0
	"Q(0)"	2883.57	2871.69	
			2871.48	12.1
			2871.31	
			2870.97	
	P(1)	2863.0231	2852.07	
			2851.55	11.5
			2850.89	

$(HCl)_2$ ν_2^- region
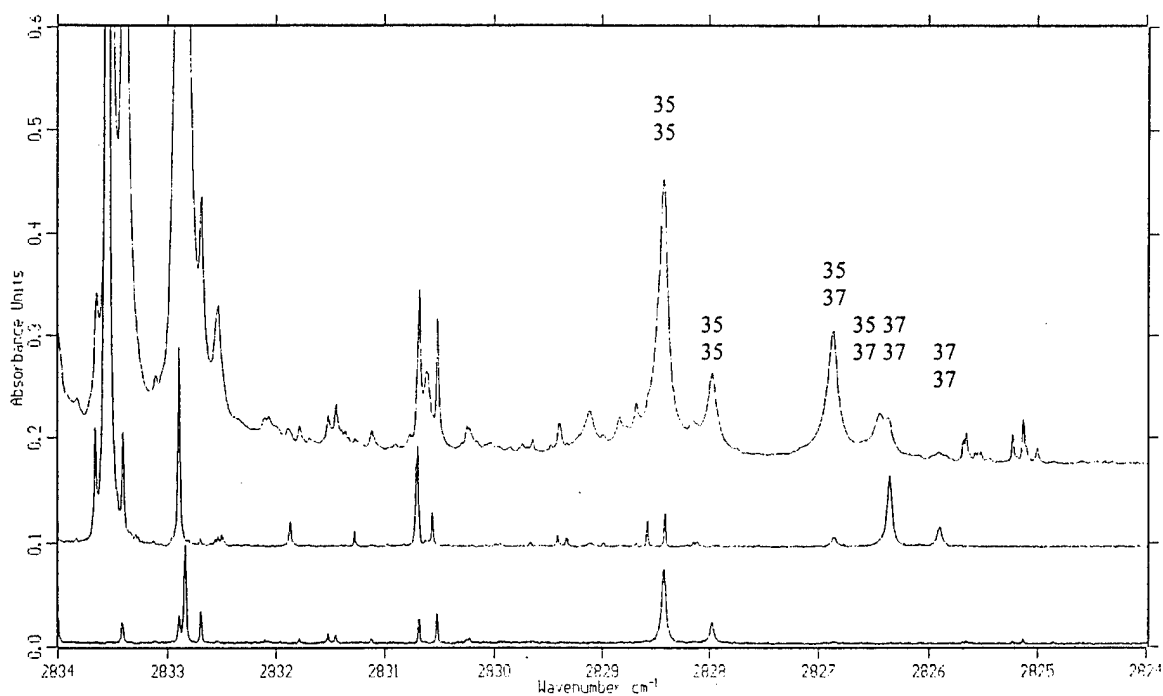
st27067.10	annealed	T=2.4K	494 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $H^{37}Cl$
st27079.11	annealed	T=2.4K	90 PPM $H^{35}Cl$

$(HCl)_2$ ν_2^- region

st27061.11	annealed	T=2.4K	88 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $H^{37}Cl$
st27079.11	annealed	T=2.4K	90 PPM $H^{35}Cl$

$(HCl)_2$ ν_1^+ region
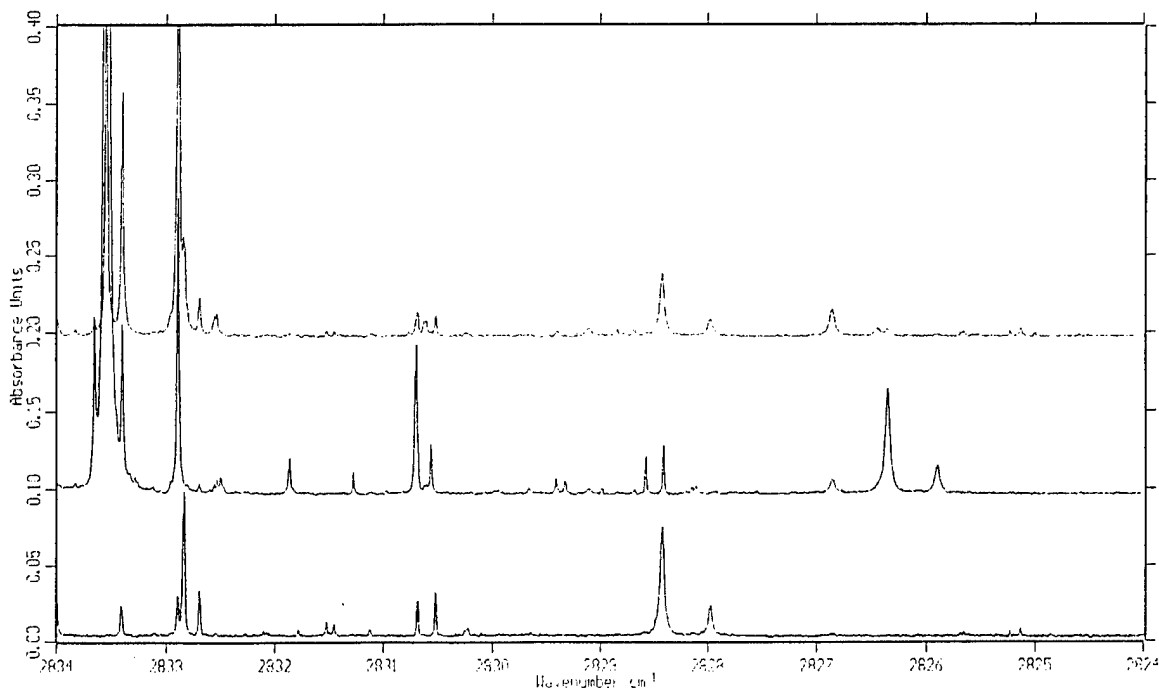
st27061.11   annealed   T=2.4K   88 PPM HCl
st27103.6   annealed   T=2.4K   94 PPM $H^{37}Cl$
st27079.11   annealed   T=2.4K   90 PPM $H^{35}Cl$
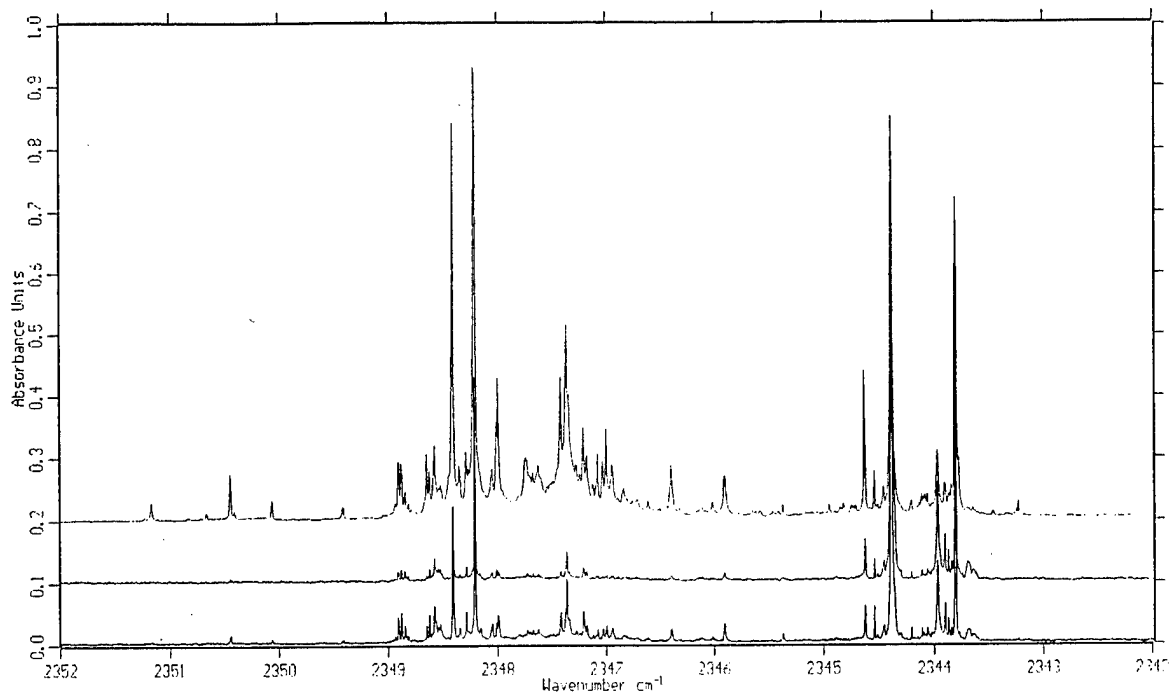
ST27103.6

$(HCl)_2$ ν_1^+ region
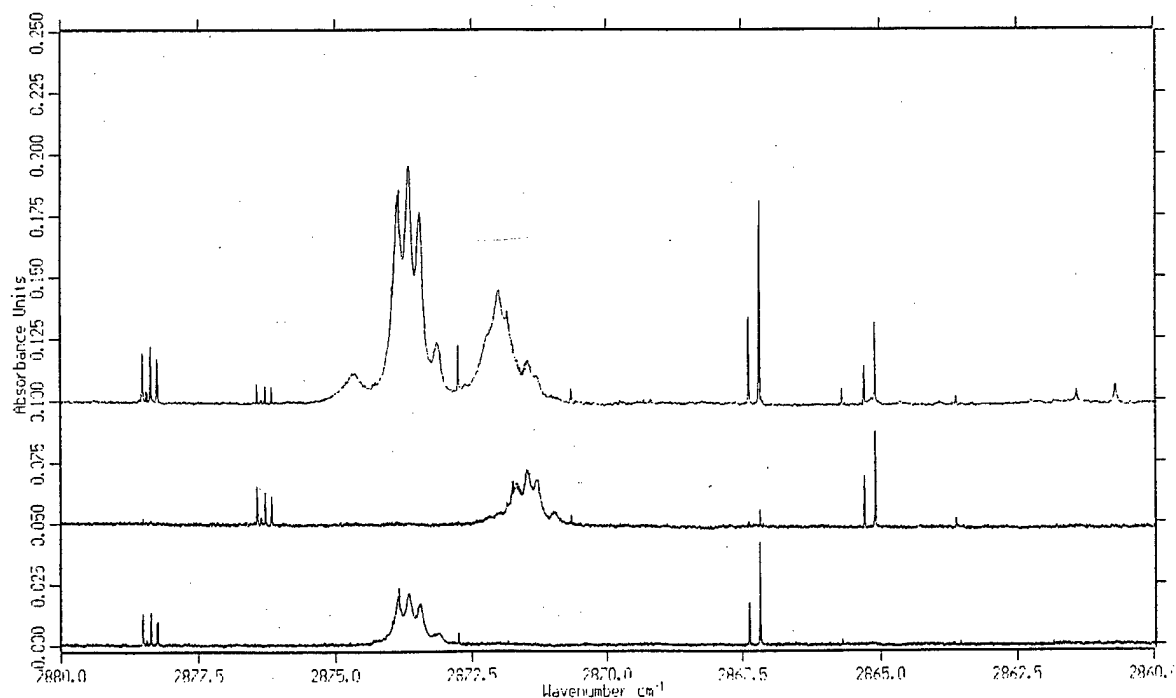
st27061.11   annealed   T=2.4K   88 PPM HCl
st27097.6   annealed   T=2.4K   33 PPM $H^{37}Cl$
st27073.17   annealed   T=2.4K   30 PPM $H^{35}Cl$

$(HCl)_2 \; \nu_1^{+}$ region

st27067.10	annealed	T=2.4K	494 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $H^{37}Cl$
st27085.9	annealed	T=2.4K	284 PPM $H^{35}Cl$

$(HCl)_n$

st27067.10	annealed	T=2.4K	494 PPM HCl
st27103.6	annealed	T=2.4K	94 PPM $H^{37}Cl$
st27085.9	annealed	T=2.4K	284 PPM $H^{35}Cl$

(HCl)$_3$
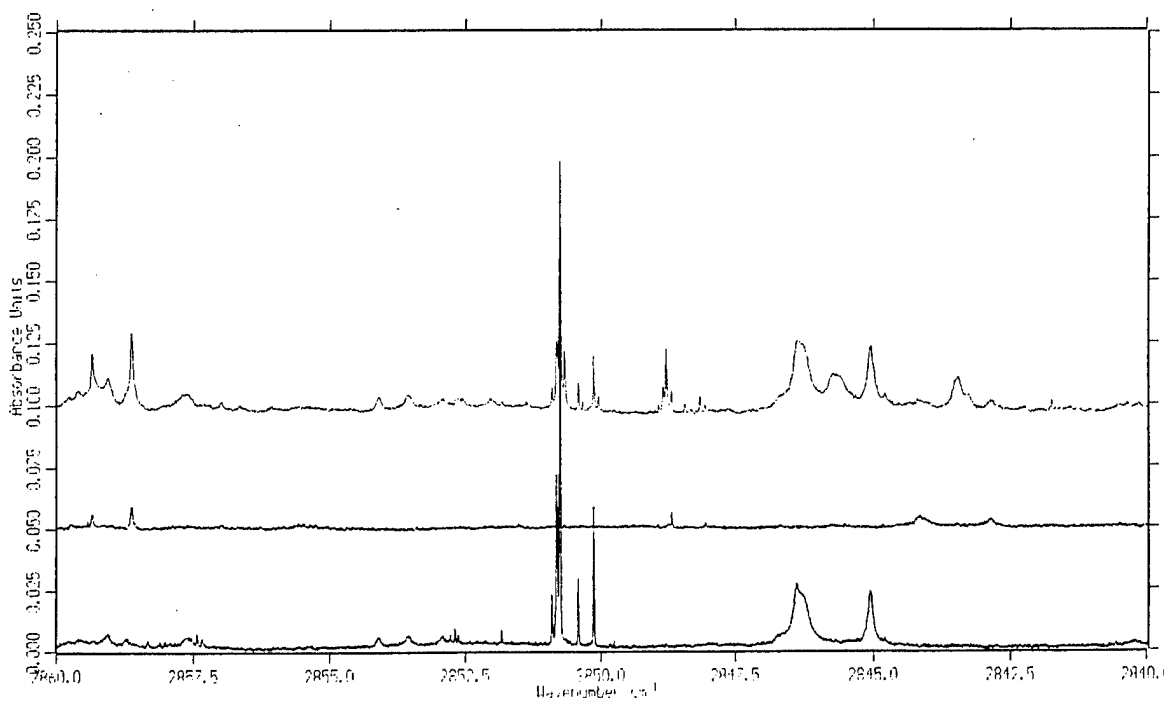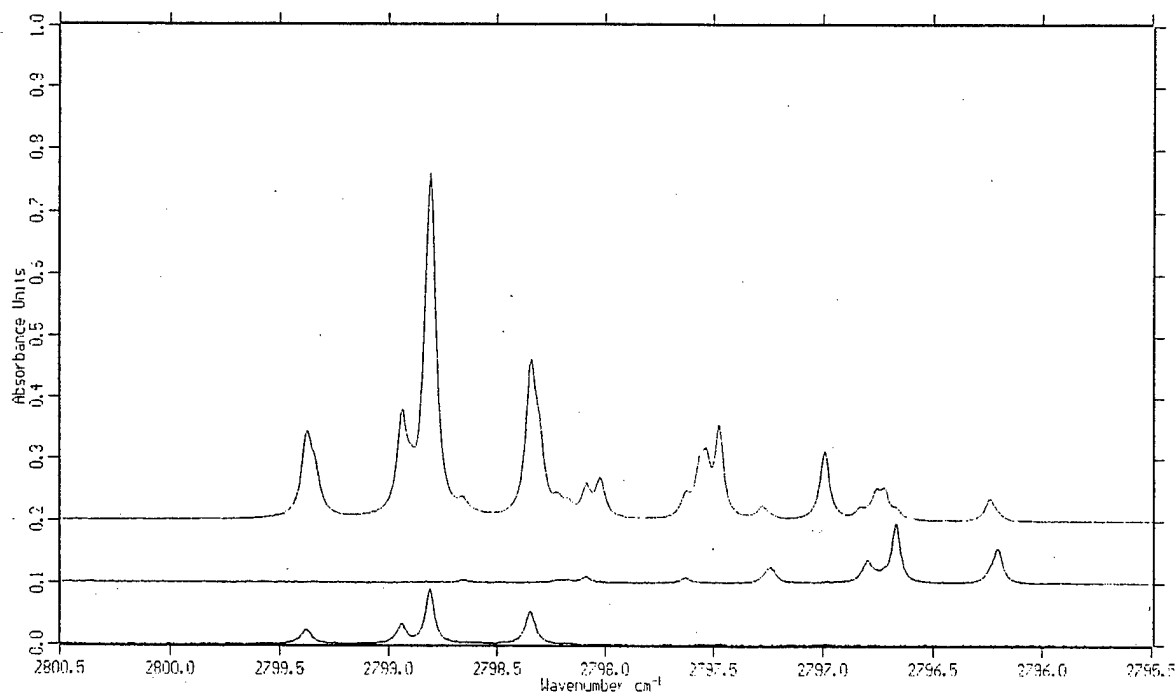
st27061.11	annealed	T=2.4K	88 PPM HCl
st27097.6	annealed	T=2.4K	33 PPM H^{37}Cl
st27073.17	annealed	T=2.4K	30 PPM H^{35}Cl

ST27061.11

ν_3 CO$_2$/(HCl)$_n$ clusters

st27061.11	annealed	T=2.4K	88 PPM HCl
st27097.6	annealed	T=2.4K	33 PPM H^{37}Cl
st27073.17	annealed	T=2.4K	30 PPM H^{35}Cl

ν_3 $CO_2/(HCl)_n$ clusters

st27067.10 annealed   T=2.4K   494 PPM HCl
st27103.6   annealed   T=2.4K   94 PPM $H^{37}Cl$
st27085.9   annealed   T=2.4K   284 PPM $H^{35}Cl$

$HF-HCl/pH_2$
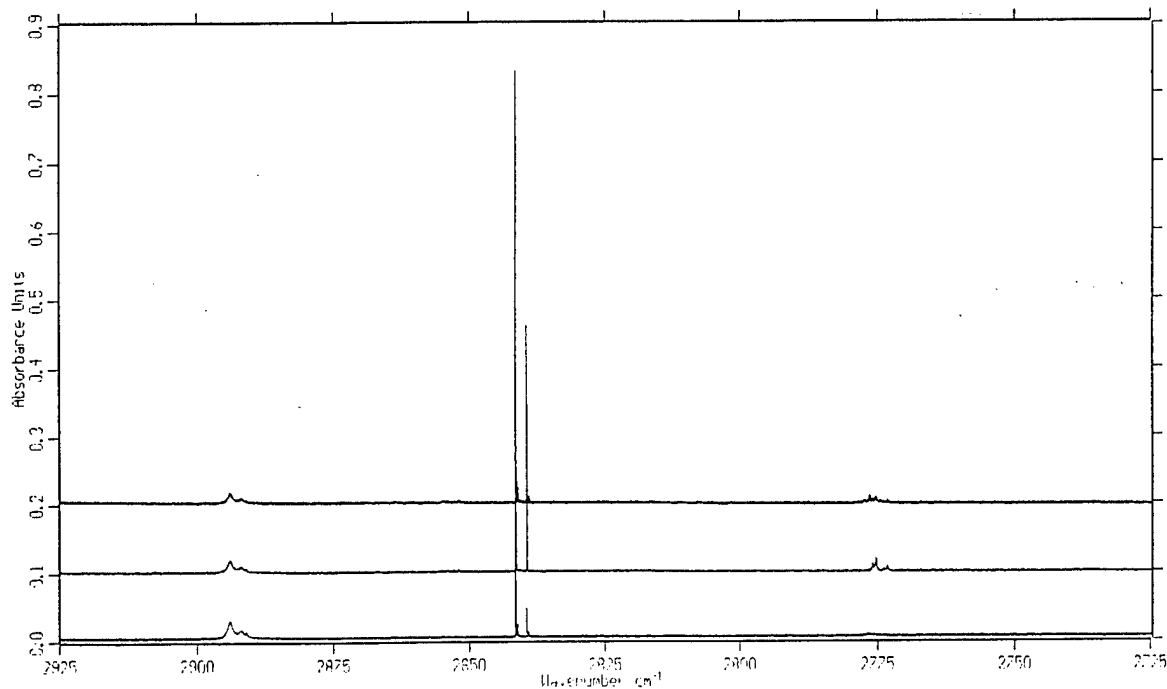
st27115.15   annealed   T=2.4K
st27115.13   annealing   T=4.8K
st27115.9   as deposited T=2.4K   123 PPM HF/pH_2 d≈3mm   resolution = 0.005 cm^{-1}

CO$_2$-HF/pH$_2$
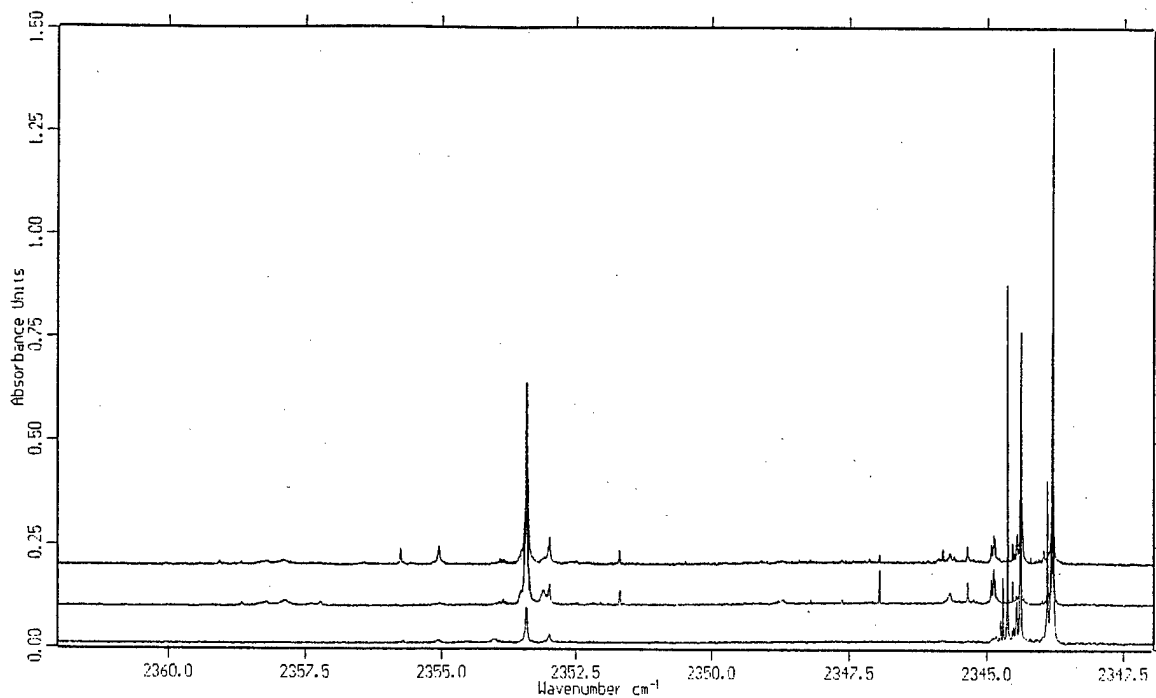
st27115.15   annealed   T=2.4K
st27115.13   annealing   T=4.8K
st27115.9   as deposited T=2.4K   123 PPM HF/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

ST27115.9

27 ~~PPM~~ *ppm* HF/pH$_2$ d≈3mm
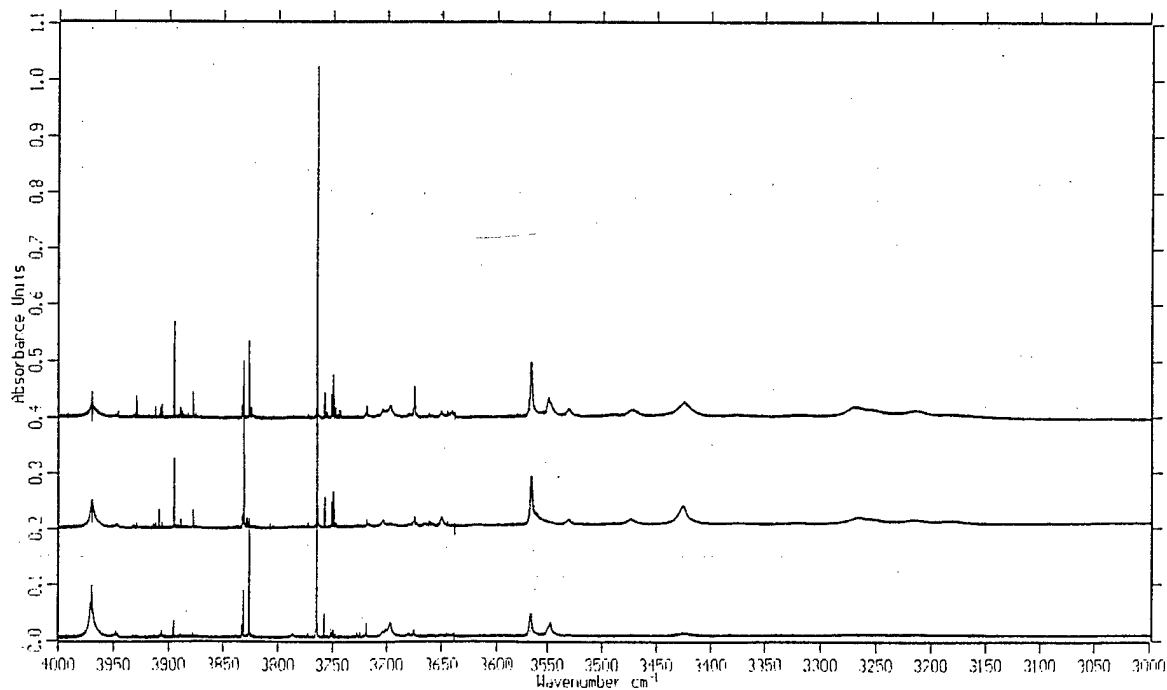
st27121.9   annealed   T=2.4K
st27121.7   annealing   T=4.8K
st27121.5   as deposited T=2.4K   resolution = 0.005 cm^{-1}

HF-HCl/pH$_2$
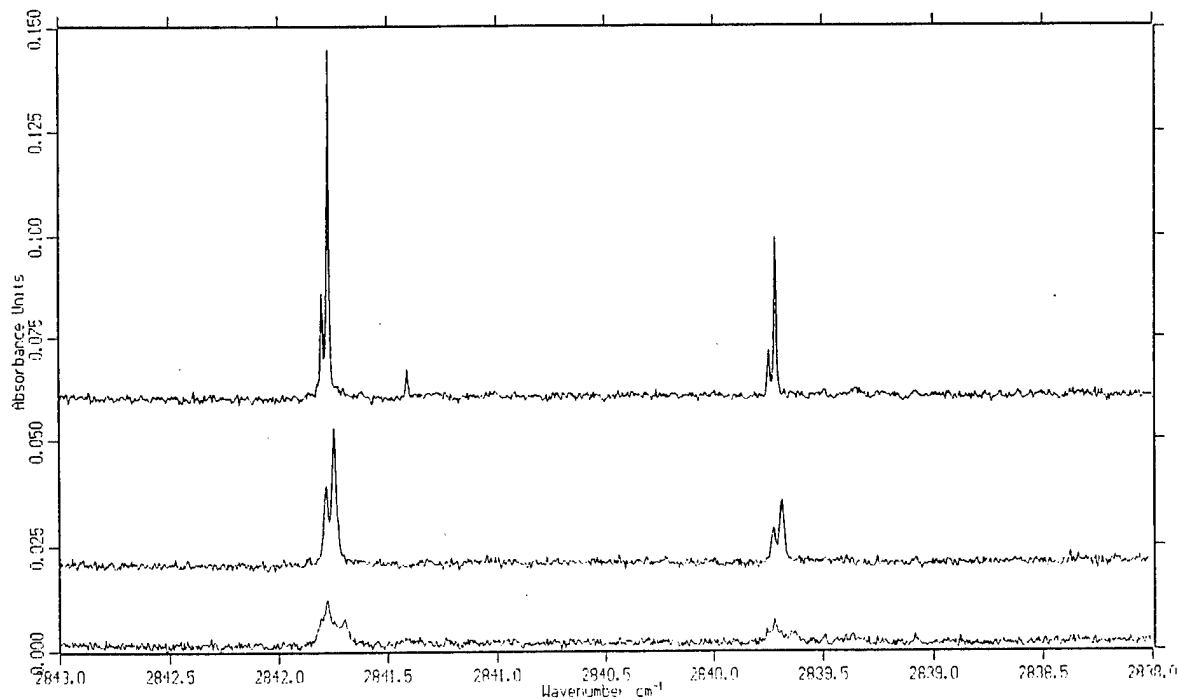
st27121.9   annealed   T=2.4K
st27121.7   annealing   T=4.8K
st27121.5   as deposited T=2.4K   27 PPM HF/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

91 ~~PPM~~ *ppm* HF/pH$_2$ d≈3mm
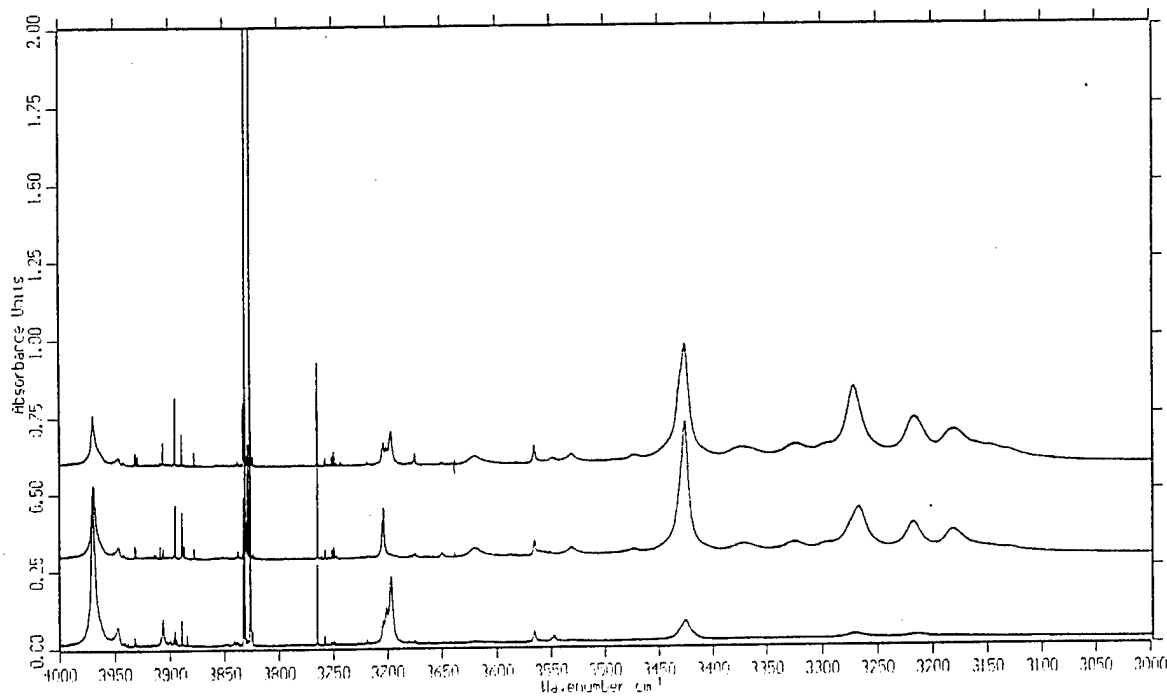
st27127.9   annealed   T=2.4K
st27127.7   annealing   T=4.8K
st27127.5   as deposited T=2.4K   resolution = 0.005 cm^{-1}

HF-HCl/pH$_2$
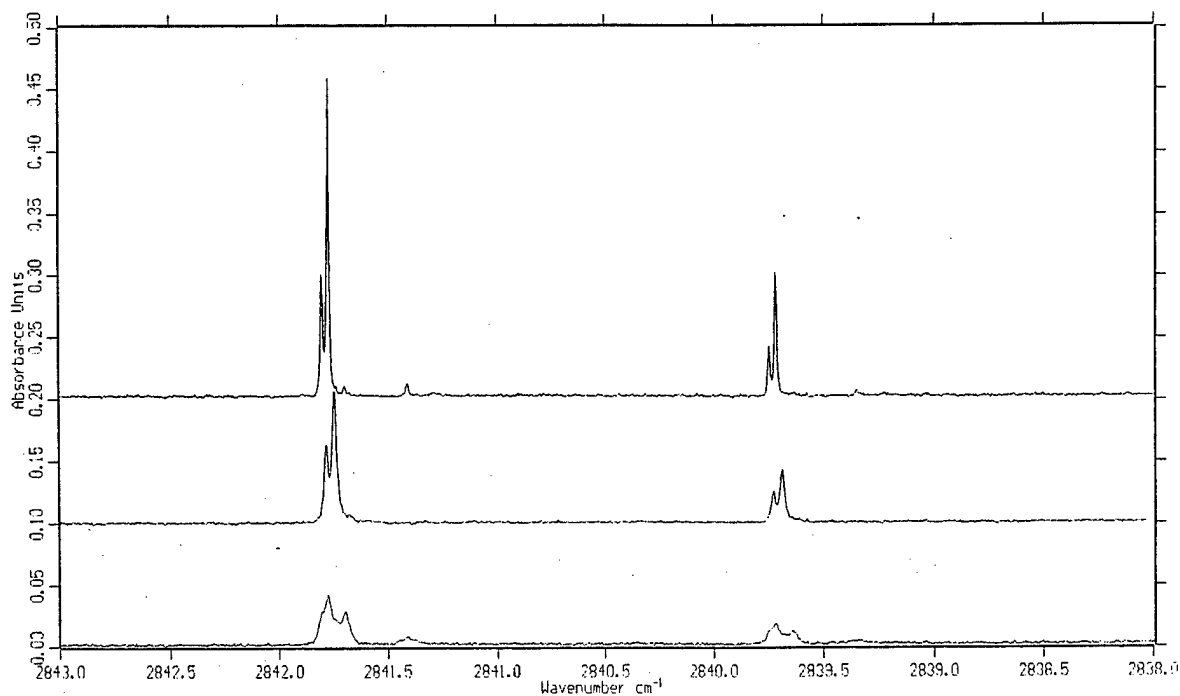
st27127.9	annealed	T=2.4K
st27127.7	annealing	T=4.8K
st27127.5	as deposited T=2.4K

91 PPM HF/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

ST27127.5

268 ~~PPM~~ ppm HF/pH$_2$ d≈3mm
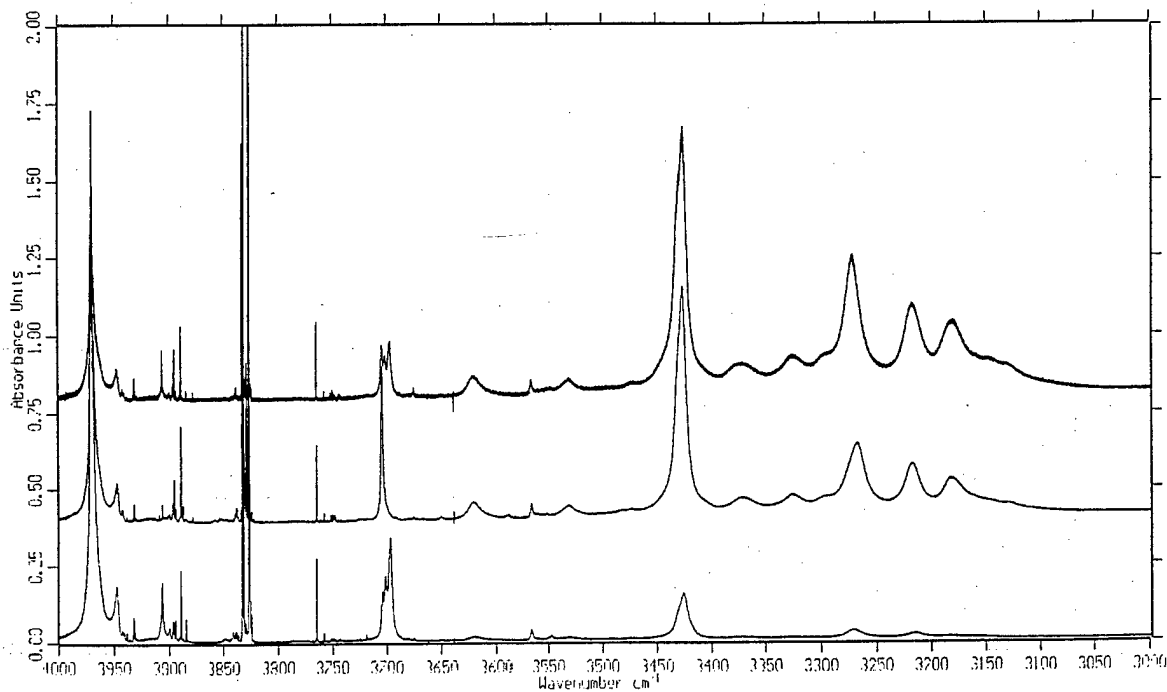
st27133.9	annealed	T=2.4K
st27133.7	annealing	T=4.8K
st27133.5	as deposited T=2.4K

resolution = 0.005 cm^{-1}

HF-HCl/pH₂
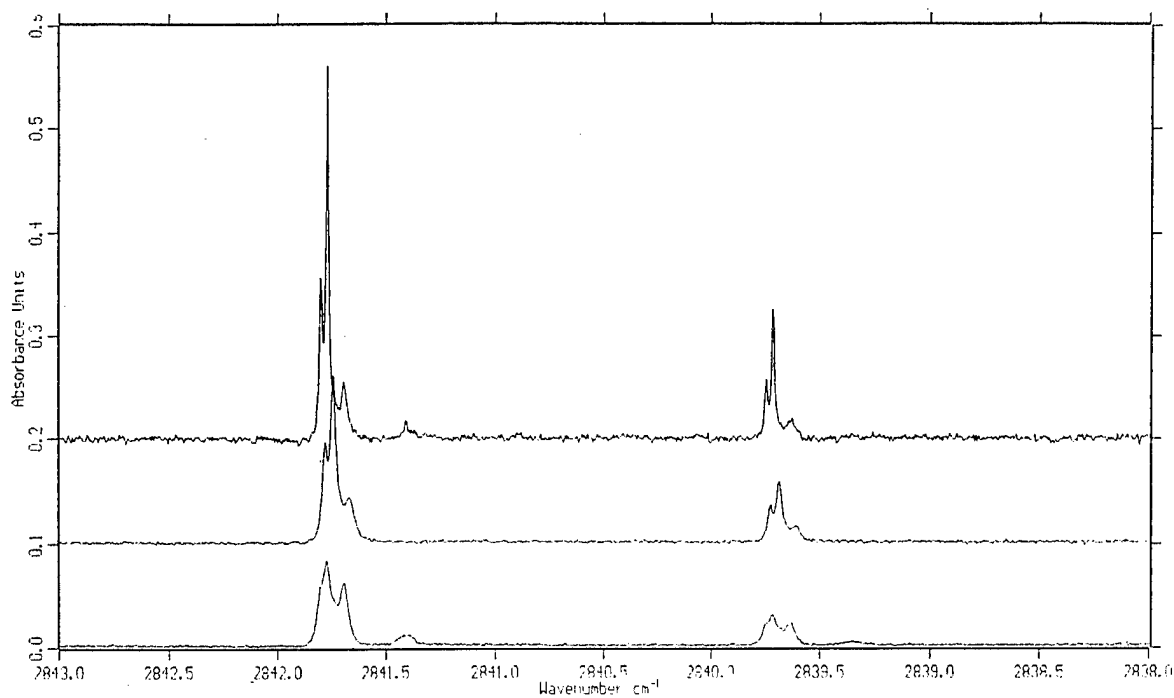
st27133.9	annealed	T=2.4K		
st27133.7	annealing	T=4.8K		
st27133.5	as deposited	T=2.4K	268 PPM HF/pH₂ d≈3mm	resolution = 0.005 cm⁻¹
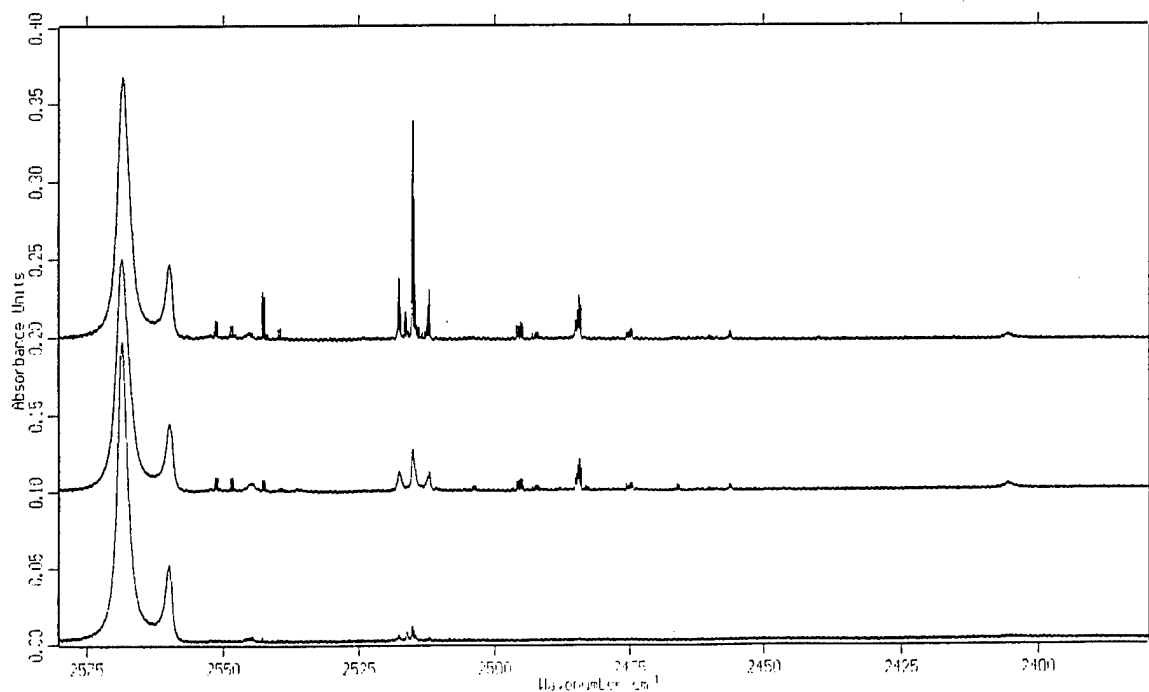
80 ~~PPM~~ *ppm* HBr/pH₂ d≈3mm

st27140.9	annealed	T=2.4K	
st27140.7	annealing	T=4.8K	
st27140.5	as deposited	T=2.4K	resolution = 0.005 cm⁻¹

HF-(HF, HCl, HBr)/pH₂

st27140.9	annealed	T=2.4K
st27140.7	annealing	T=4.8K
st27140.5	as deposited T=2.4K	80 PPM HBr/pH₂ d≈3mm	resolution = 0.005 cm⁻¹

HCl-HBr/pH₂

st27140.9	annealed	T=2.4K
st27140.7	annealing	T=4.8K
st27140.5	as deposited T=2.4K	80 PPM HBr/pH₂ d≈3mm	resolution = 0.005 cm⁻¹
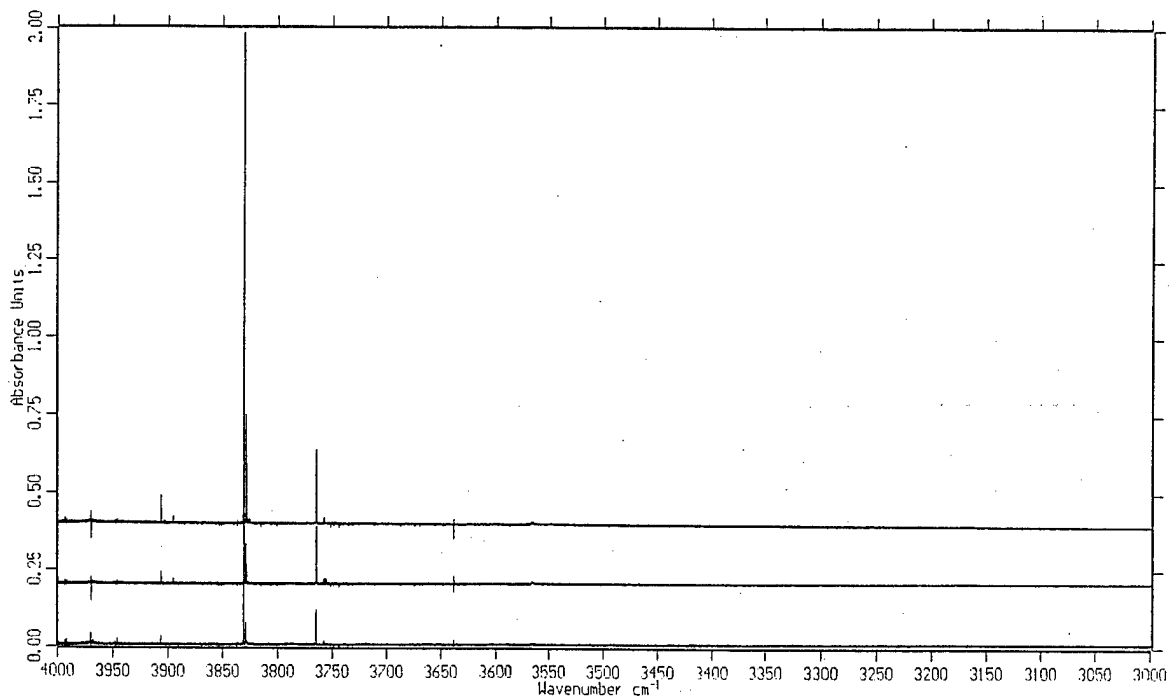
HCl-(HF, HCl, HBr)/pH$_2$

st27140.9   annealed   T=2.4K
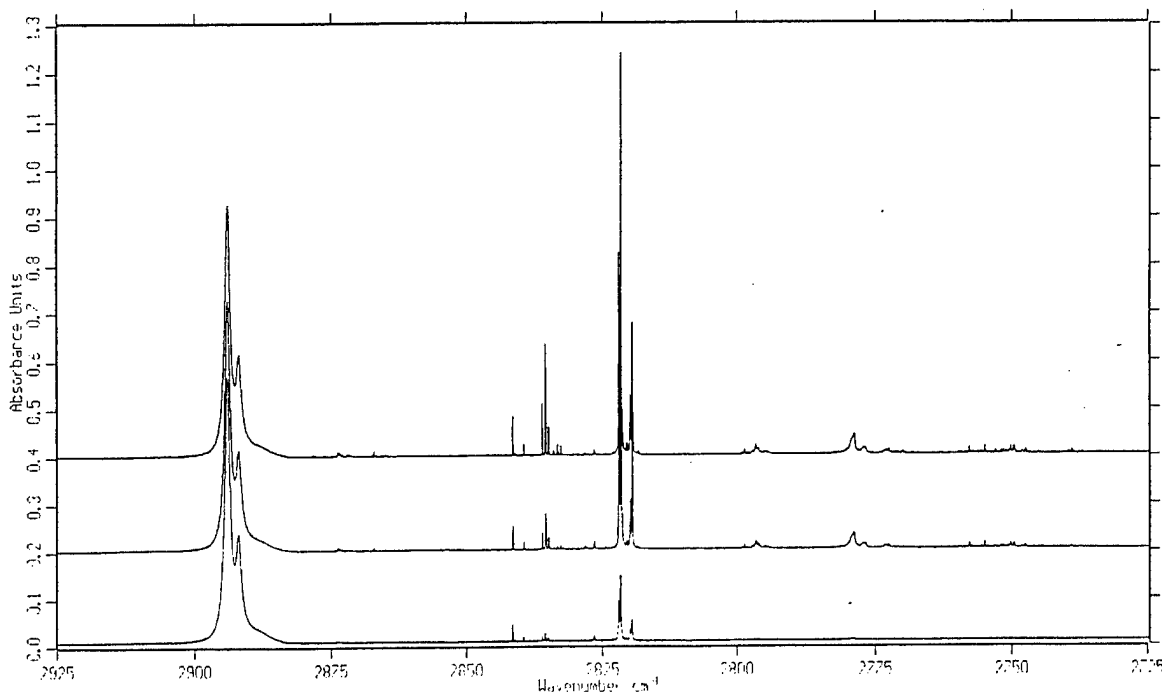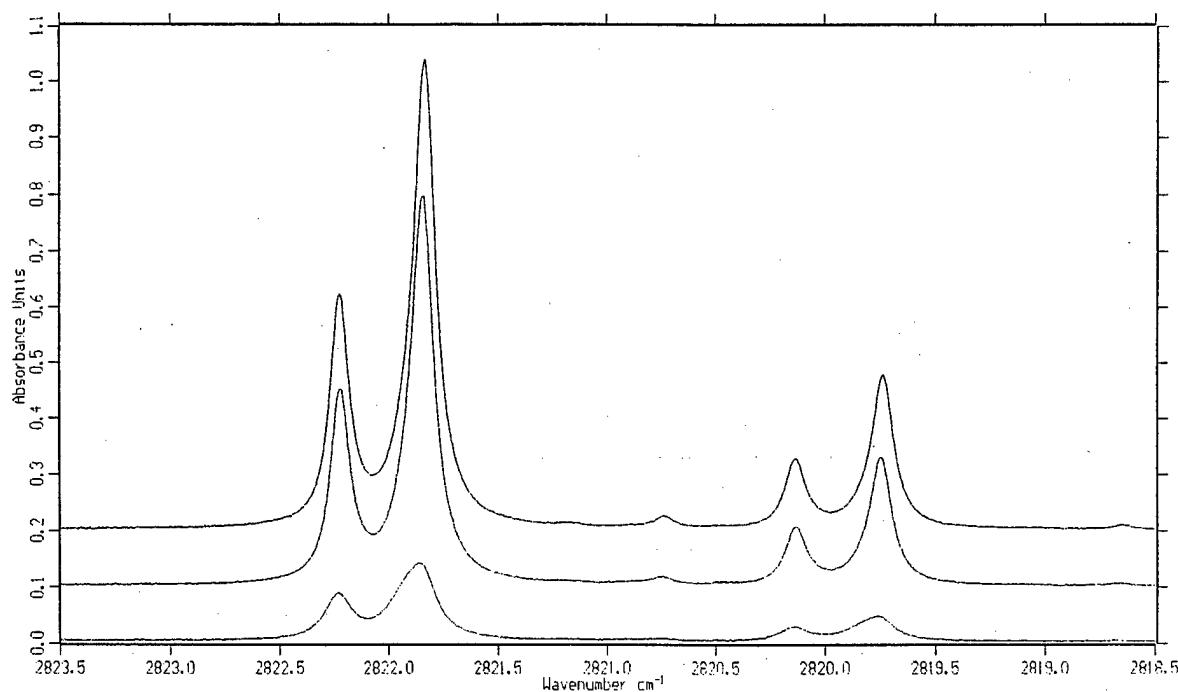st27140.7   annealing   T=4.8K
st27140.5   as deposited T=2.4K   80 PPM HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}
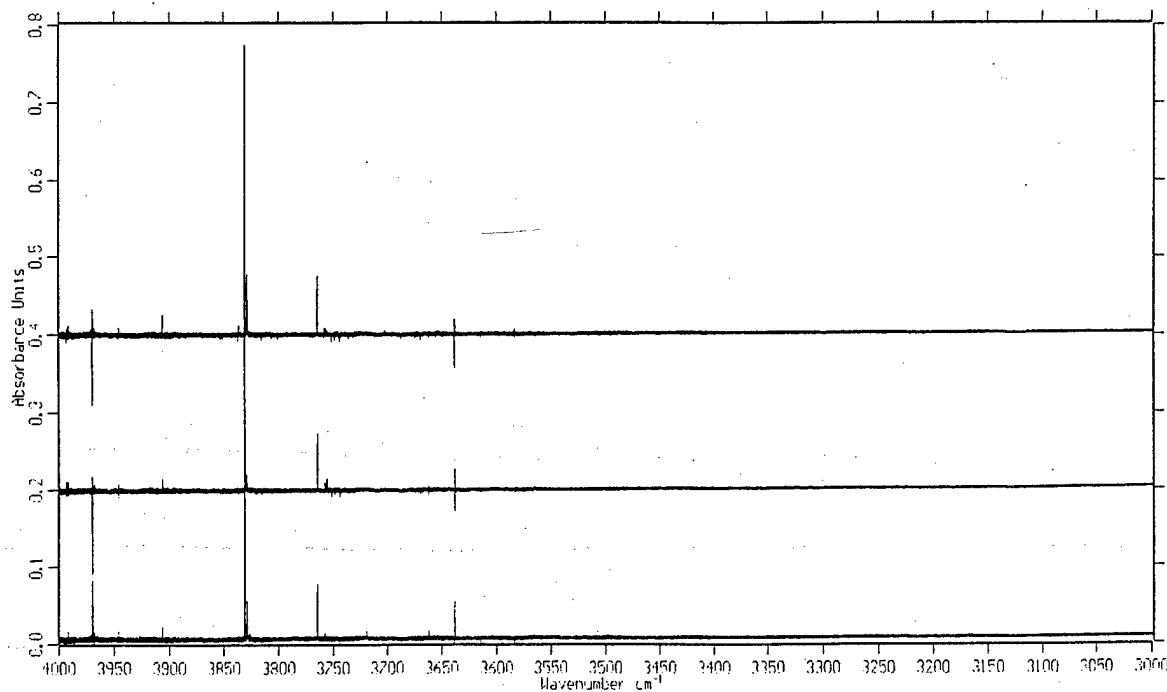   ST27140.5

HCl-(HF, HCl, HBr)/pH$_2$

st27145.9   annealed   T=2.4K
st27145.7   annealing   T=4.8K
st27145.5   as deposited T=2.4K   260 PPM HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

HCl-HBr/pH$_2$

st27145.9   annealed   T=2.4K
st27145.7   annealing   T=4.8K
st27145.5   as deposited T=2.4K   260 PPM HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}
ST27145.5

HF-(HF, HCl, HBr)/pH$_2$

st27145.9   annealed   T=2.4K
st27145.7   annealing   T=4.8K
st27145.5   as deposited T=2.4K   260 PPM HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}
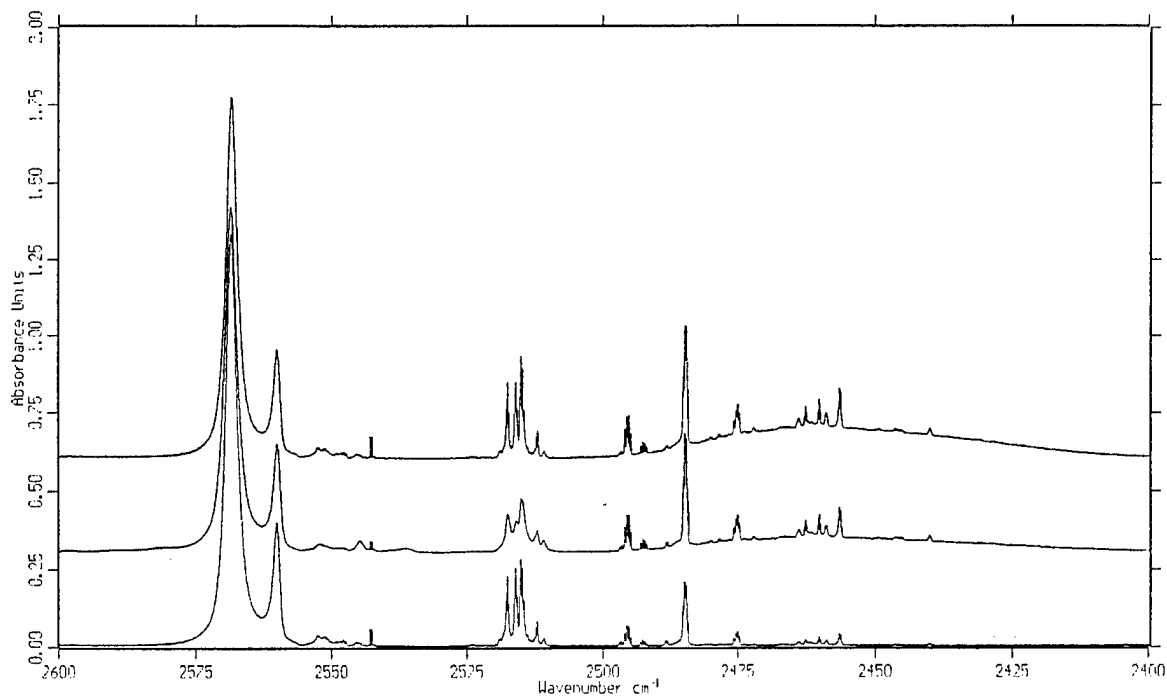
645 HBr/pH$_2$ d≈3mm

st28003.9   annealed   T=2.4K
st28003.7   annealing   T=4.8K
st28003.5   as deposited T=2.4K   resolution = 0.005 cm^{-1}

ST28003.5

HCl(HBr)$_n$/pH$_2$

st28003.9   annealed   T=2.4K
st28003.7   annealing   T=4.8K
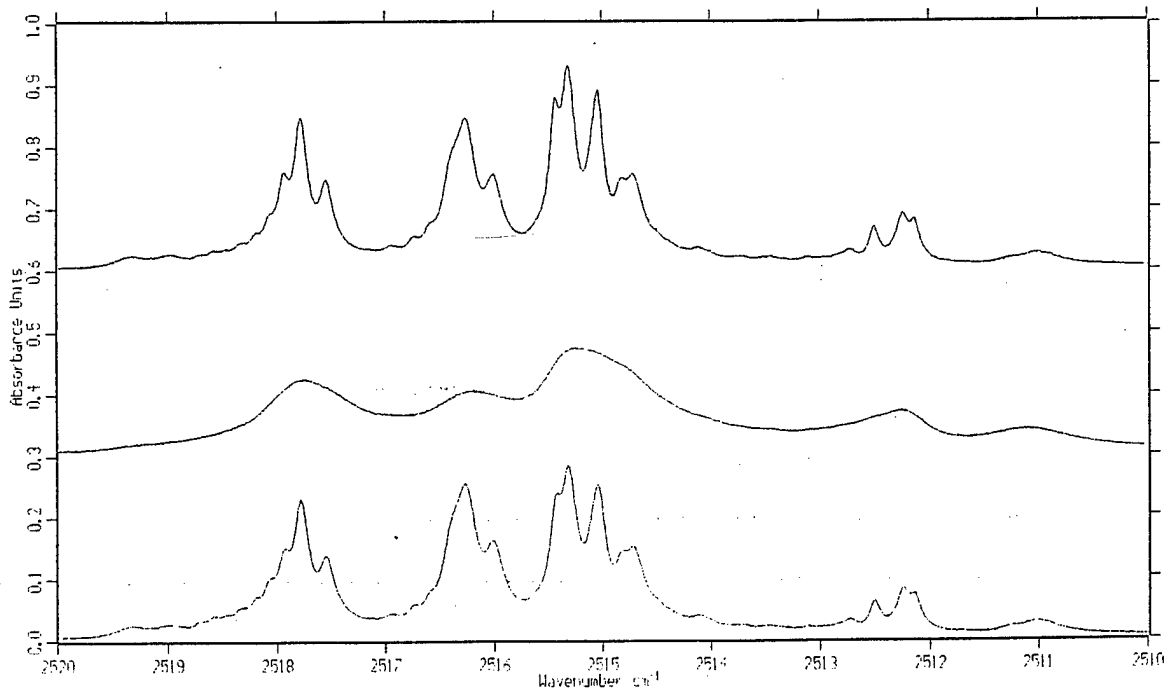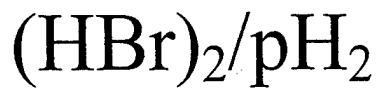st28003.5   as deposited T=2.4K   645 HBr/pH$_2$ d≈3mm   resolution = 0.005 cm^{-1}

CO$_2$(HBr)$_n$/pH$_2$

st28003.9   annealed   T=2.4K
st28003.7   annealing   T=4.8K
st28003.5   as deposited T=2.4K   645 HBr/pH$_2$ d$\approx$3mm   resolution = 0.005 cm^{-1}

ST28003.5

(HBr)$_2$/pH$_2$

st28003.9   annealed   T=2.4K
st28003.7   annealing   T=4.8K
st28003.5   as deposited T=2.4K   645 HBr/pH$_2$ d$\approx$3mm   resolution = 0.005 cm^{-1}

15 PPM H_2O/pH_2 d≈3mm

st28010.6 annealed T=2.4K
st28010.4 annealing T=4.8K
st28010.2 as deposited T=2.4K   resolution = 0.005 cm^{-1}

15 PPM H_2O/pH_2 d≈3mm

st28010.6 annealed T=2.4K
st28010.4 annealing T=4.8K
st28010.2 as deposited T=2.4K   resolution = 0.005 cm^{-1}

45 PPM H₂O/pH₂ d≈3mm

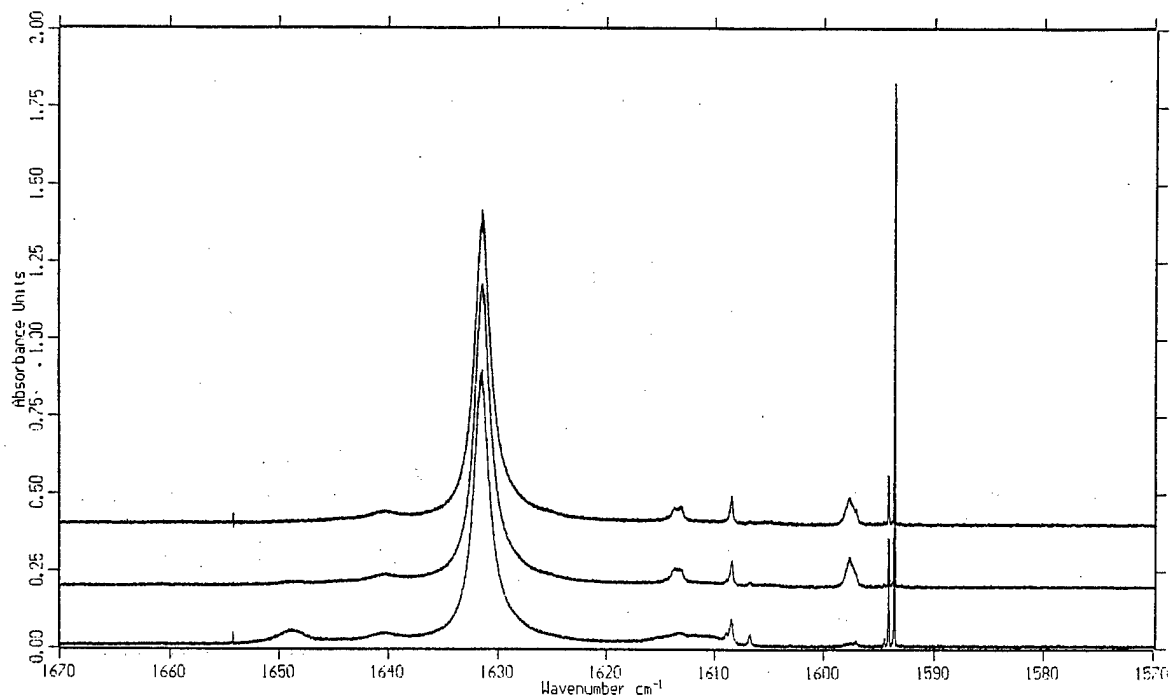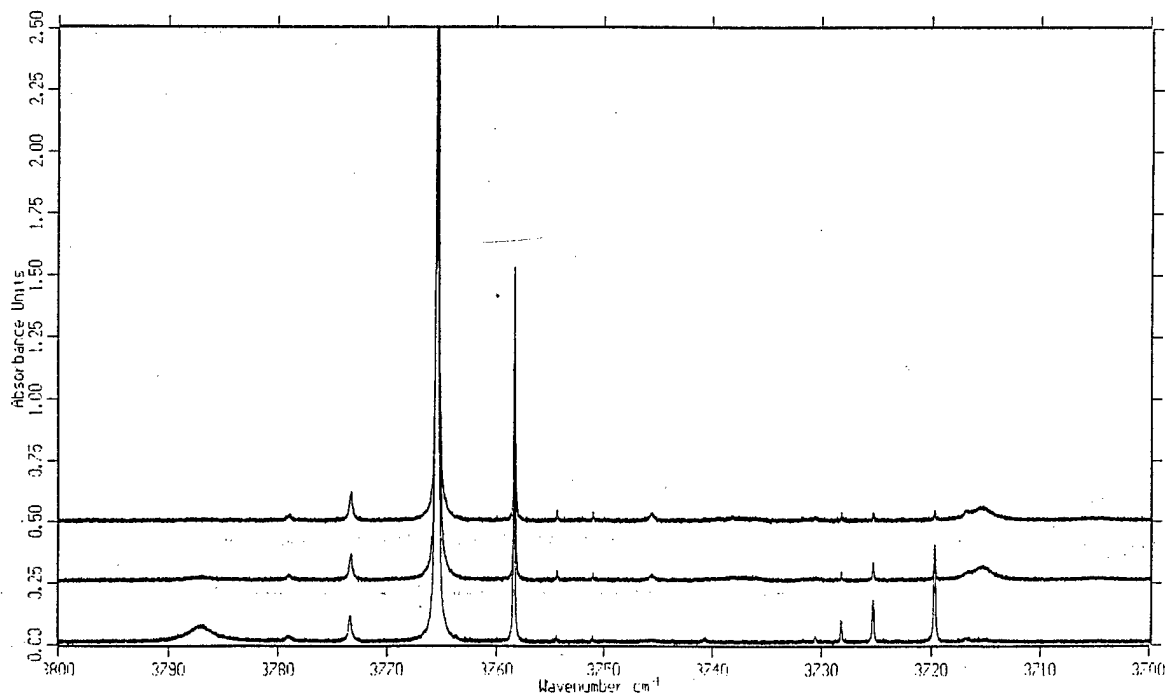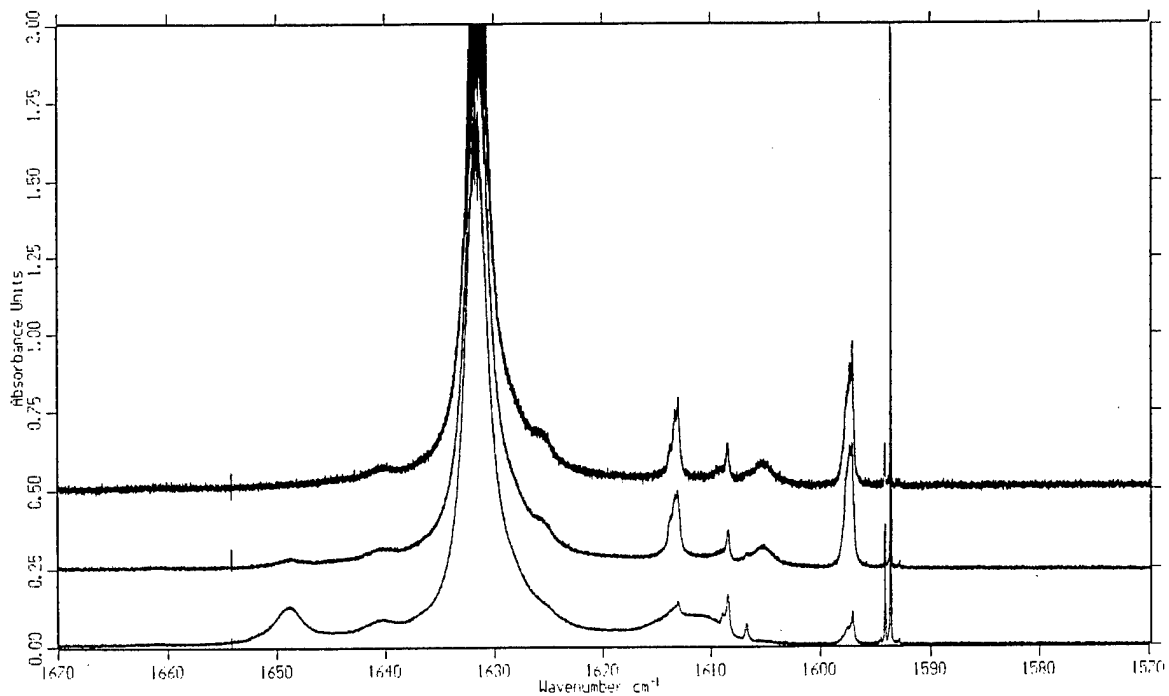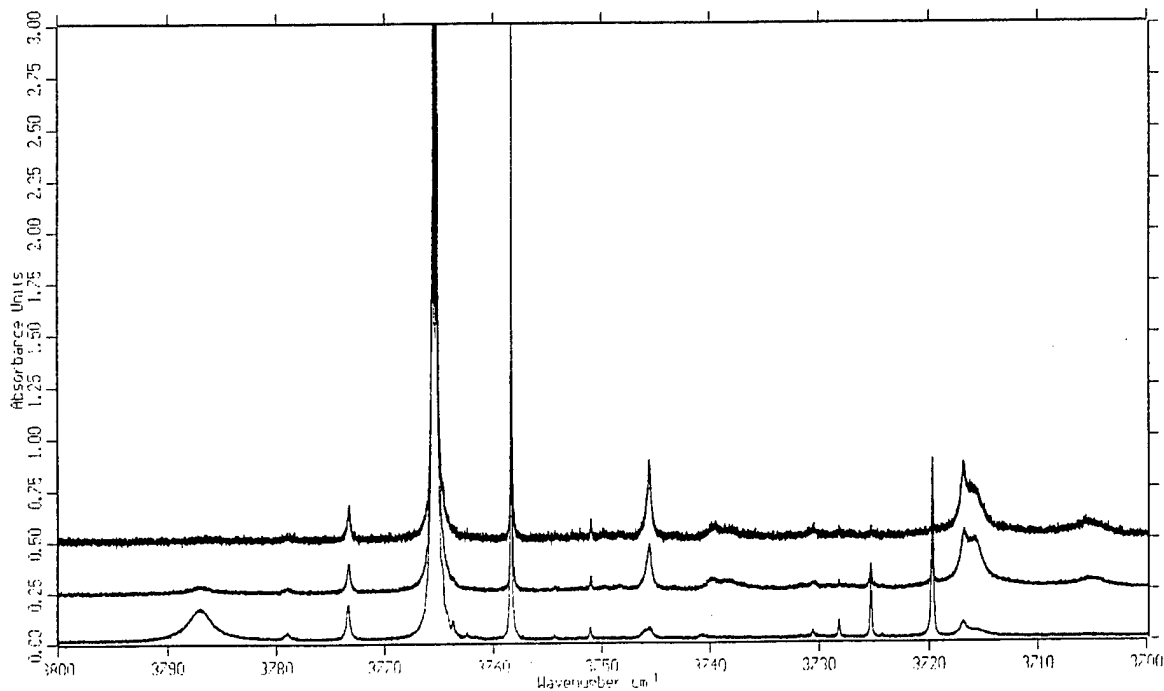$$\text{45 PPM } H_2O/pH_2 \quad d\approx 3mm$$

st28014.6	annealed	T=2.4K
st28014.4	annealing	T=4.8K
st28014.2	as deposited T=2.4K	resolution = 0.005 cm⁻¹

ST28014.2

45 PPM H₂O/pH₂ d≈3mm

$$\text{45 PPM } H_2O/pH_2 \quad d\approx 3mm$$

st28014.6	annealed	T=2.4K
st28014.4	annealing	T=4.8K
st28014.2	as deposited T=2.4K	resolution = 0.005 cm⁻¹

138 PPM H₂O/pH₂ d≈3mm

$$138 \text{ PPM H}_2\text{O/pH}_2 \quad d\approx3\text{mm}$$

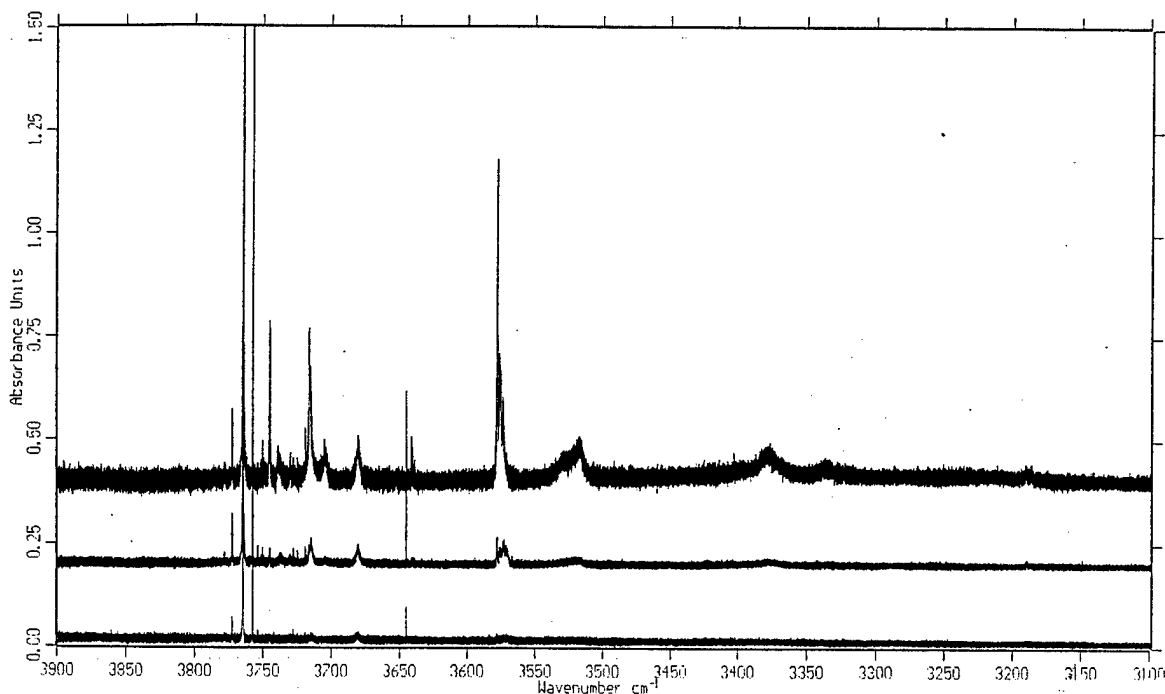|		
st28018.6	annealed	T=2.4K
st28018.4	annealing	T=4.8K
st28018.2	as deposited T=2.4K	resolution = 0.005 cm⁻¹

ST28018.3

138 PPM H₂O/pH₂ d≈3mm

st28018.6	annealed	T=2.4K
st28018.4	annealing	T=4.8K
st28018.2	as deposited T=2.4K	resolution = 0.005 cm⁻¹

H₂O clusters in pH₂

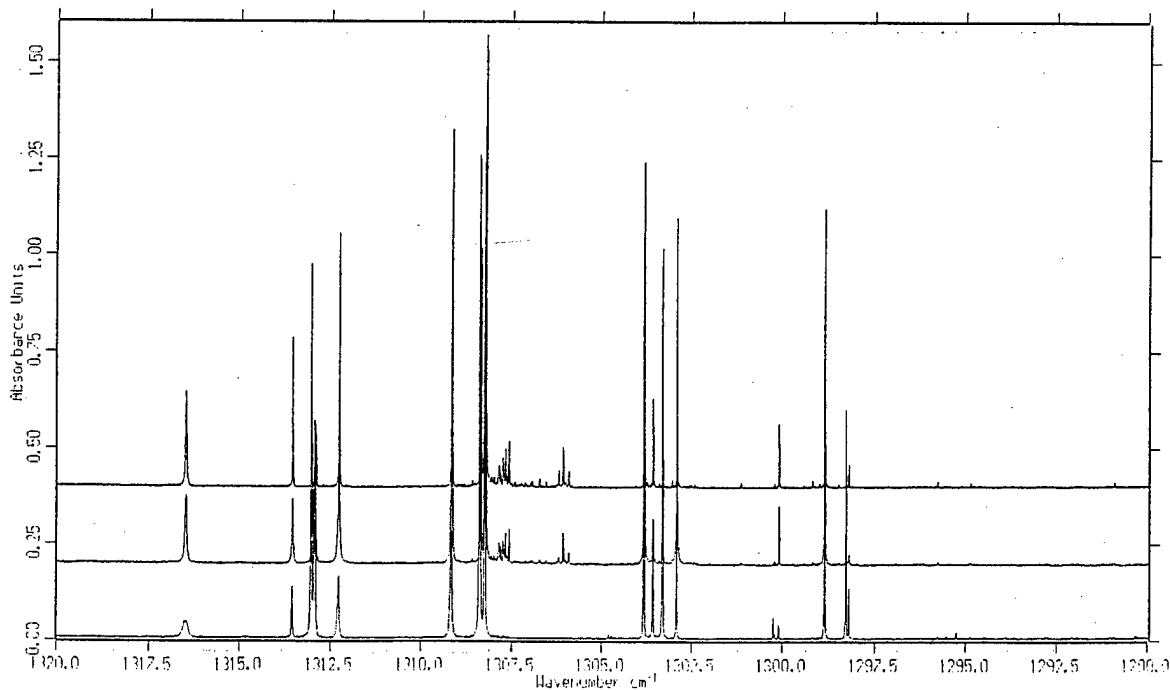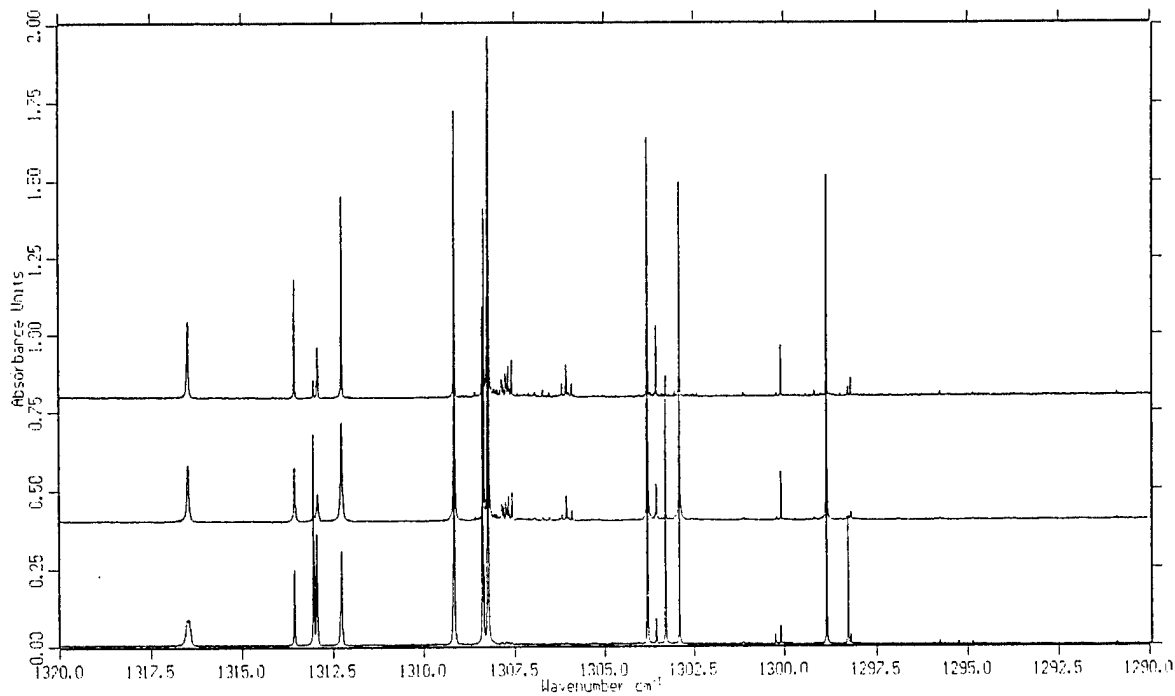|			
st28018.6	annealed	T=2.4K	138 PPM H₂O/pH₂
st28014.6	annealed	T=2.4K	45 PPM H₂O/pH₂
st28010.6	annealed	T=2.4K	15 PPM H₂O/pH₂ resolution = 0.005 cm⁻¹

ST28010.6

56 PPM CH₄/pH₂ d≈0.7mm

st28022.20	annealed	T=2.4K
st28022.19	annealing	T=4.8K
st28022.18	as deposited	T=2.4K resolution = 0.005 cm⁻¹

200 PPM CH$_4$/pH$_2$ d≈0.2mm

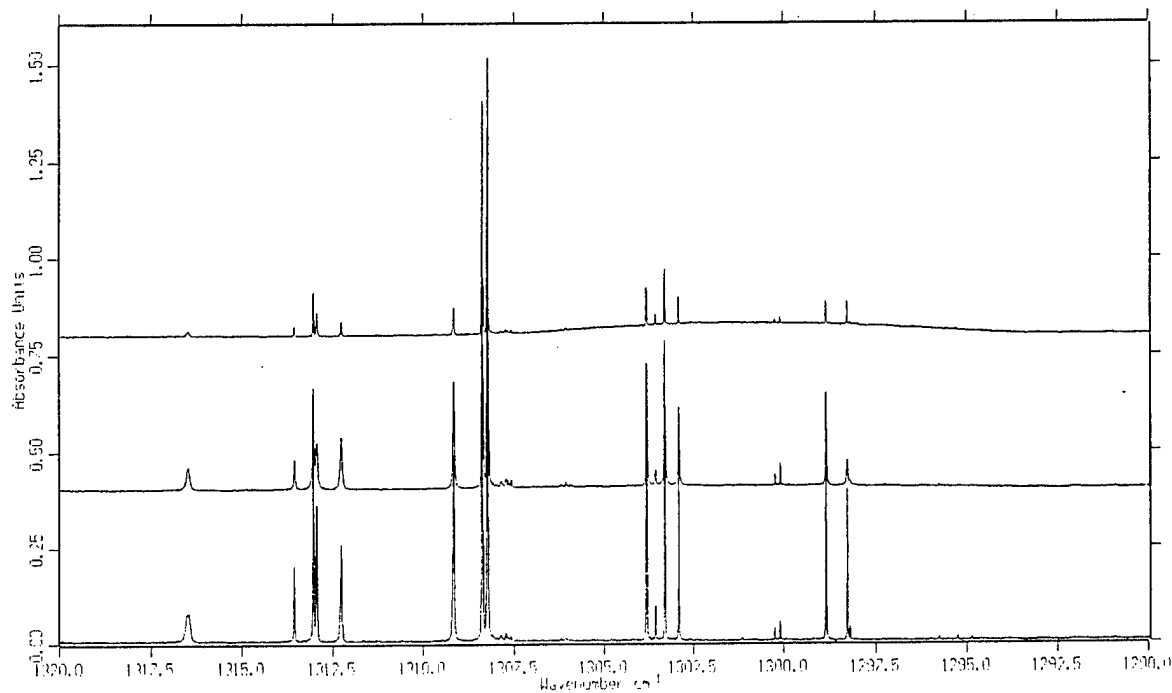Absorbance Units

Wavenumber cm⁻¹

st28026.21   annealed   T=2.4K
st28026.20   annealing   T=4.8K
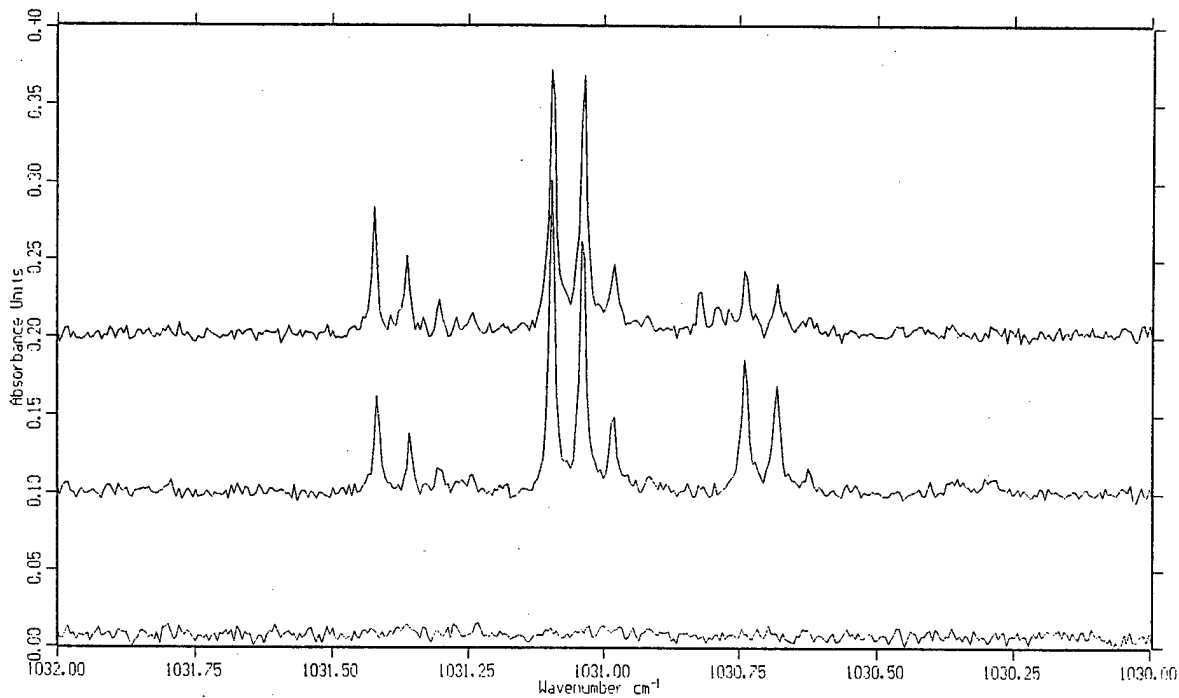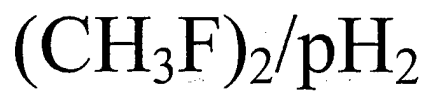st28026.19   as deposited T=2.4K   resolution = 0.005 cm⁻¹

ST28026.19

550 PPM CH$_4$/pH$_2$ d≈0.05mm

Absorbance Units

Wavenumber cm⁻¹

st28030.14   annealed   T=2.4K
st28030.13   annealing   T=4.8K
st28030.12   as deposited T=2.4K   resolution = 0.005 cm⁻¹

(CH₃F)₂/pH₂

st28039.11   annealed   T=2.4K
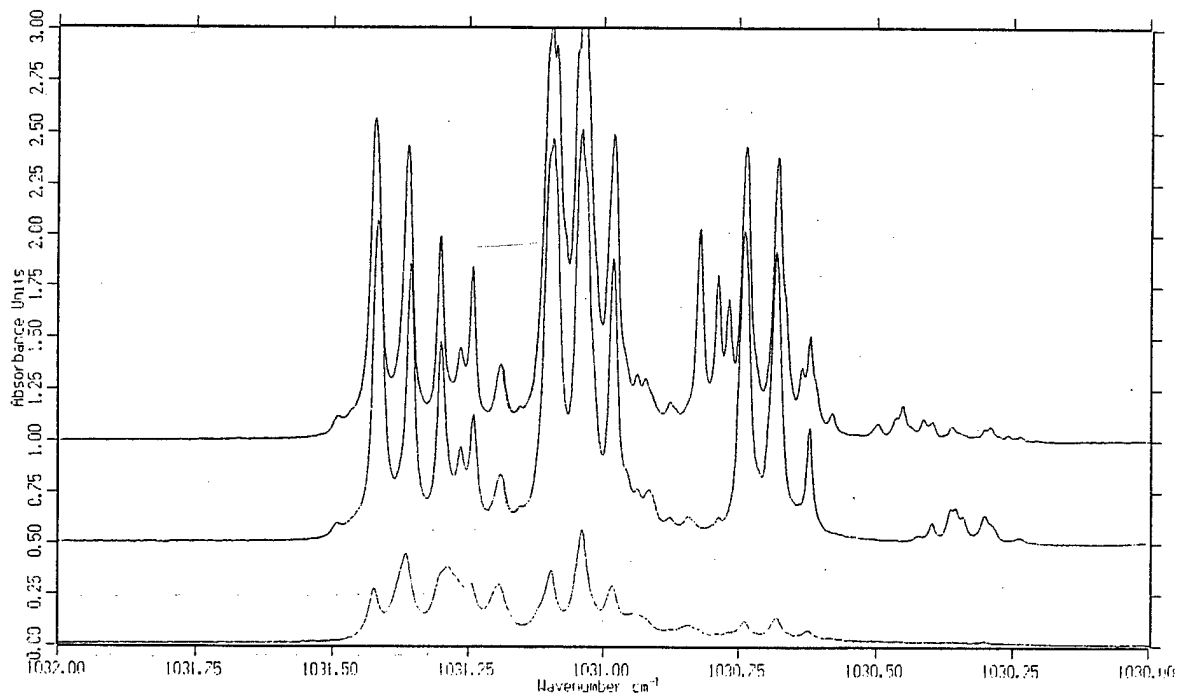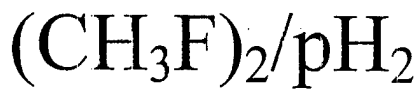st28039.9   annealing   T=4.8K
st28039.5   as deposited T=2.4K   10 PPM CH₃F/pH₂   resolution = 0.005 cm⁻¹

ST28039.5

(CH₃F)₂/pH₂

st28048.11   annealed   T=2.4K
st28048.7   annealing   T=4.8K
st28048.3   as deposited T=2.4K   91 PPM CH₃F/pH₂   resolution = 0.005 cm⁻¹

6 PPM CH₃F/pH₂ d≈3mm

$6\ \text{PPM}\ CH_3F/pH_2\ \ d\approx3mm$
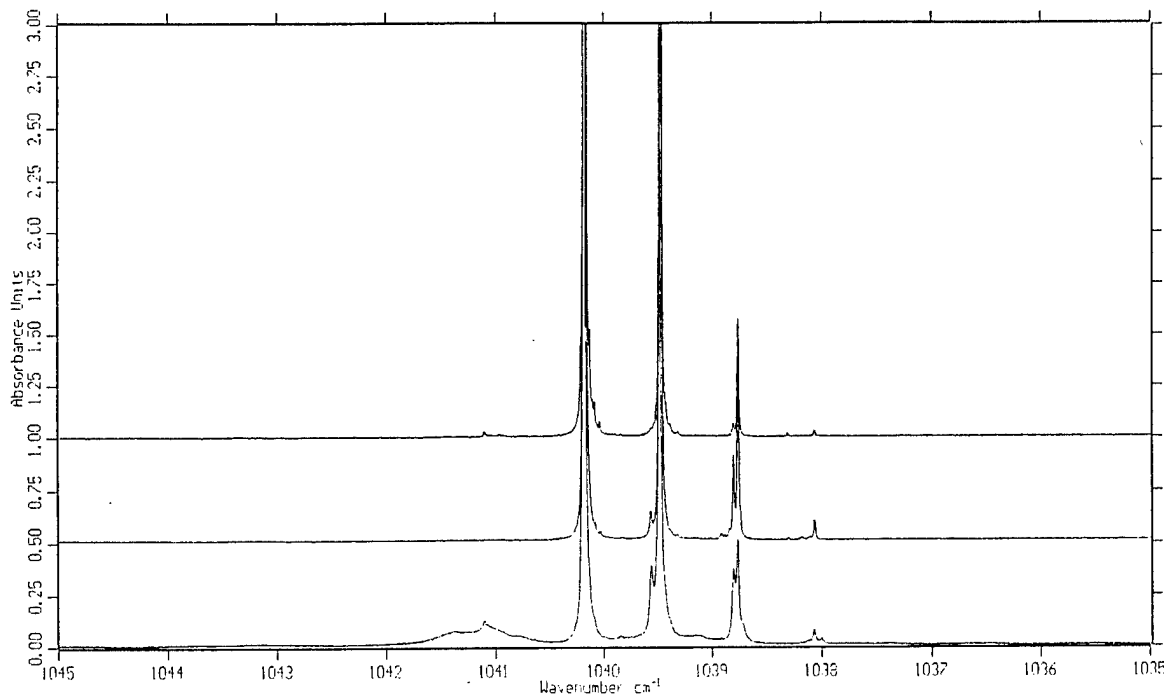
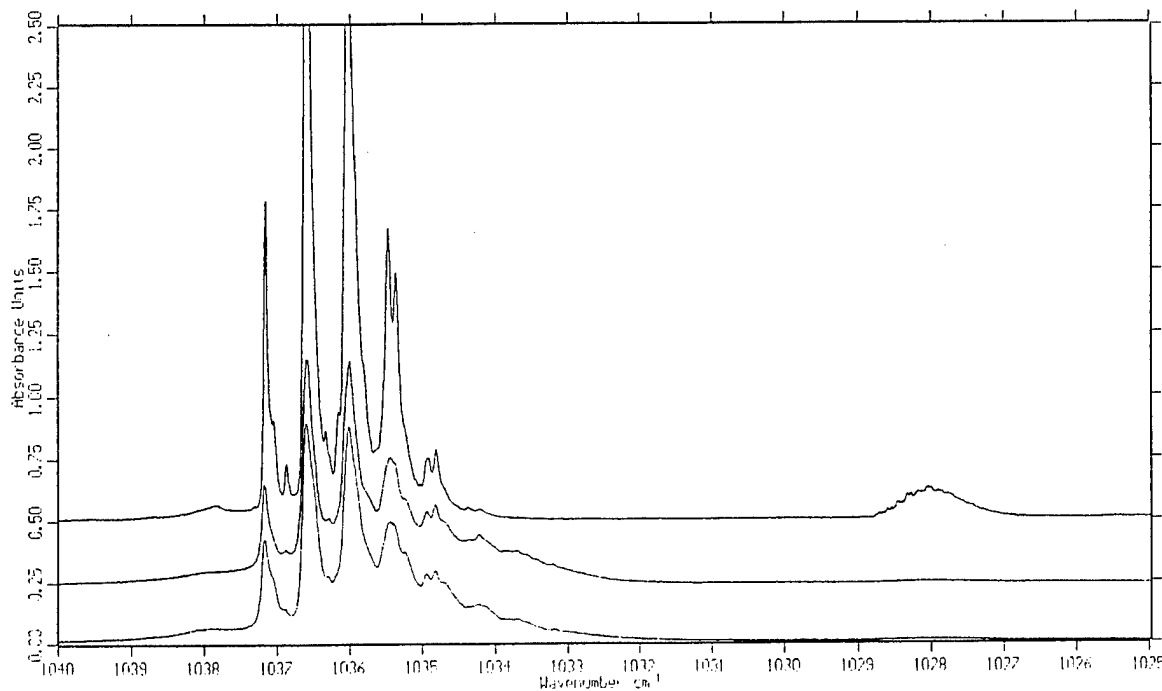st28052.10   annealed   T=2.4K
st28052.6   annealing   T=4.8K
st28052.2   as deposited T=2.4K   resolution = 0.005 cm⁻¹
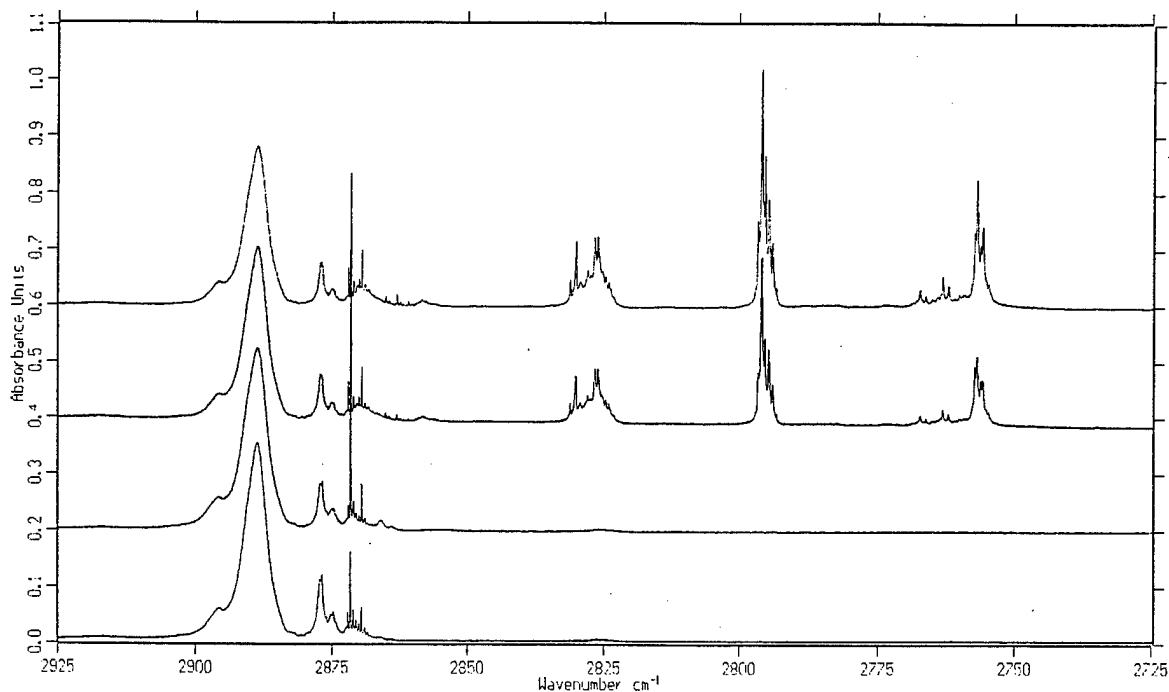
ST28052.2

33 PPM CH₃F/oD₂ d≈2mm

$33\ \text{PPM}\ CH_3F/oD_2\ \ d\approx2mm$

st28073.11   flash annealed to 10K   T=2.4K
st28073.7   annealing   T=4.8K
st28073.3   as deposited T=2.4K   resolution = 0.005 cm⁻¹

93 PPM HCl/oD$_2$ d$\approx$2mm
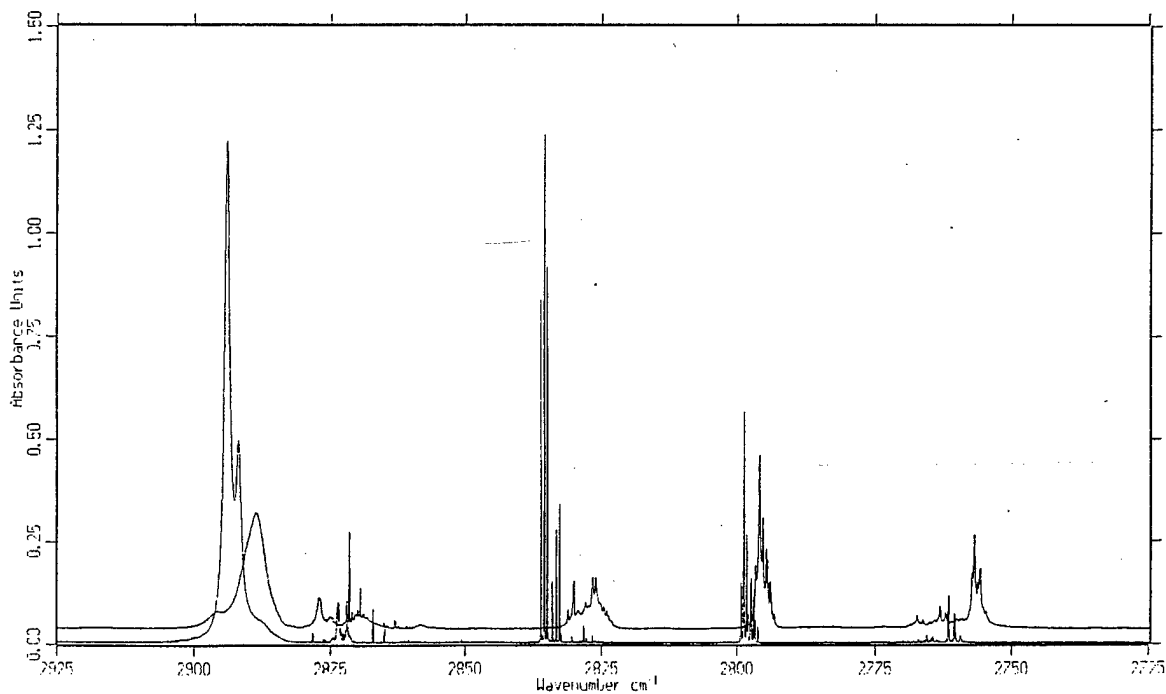

st28079.7   2nd flash annealing   T=2.4K   st28079.3   annealing   T=4.8K
st28079.5   flash annealed to 10K   T=2.4K   st28079.1   as deposited T=2.4K   resolution = 0.005 cm^{-1}
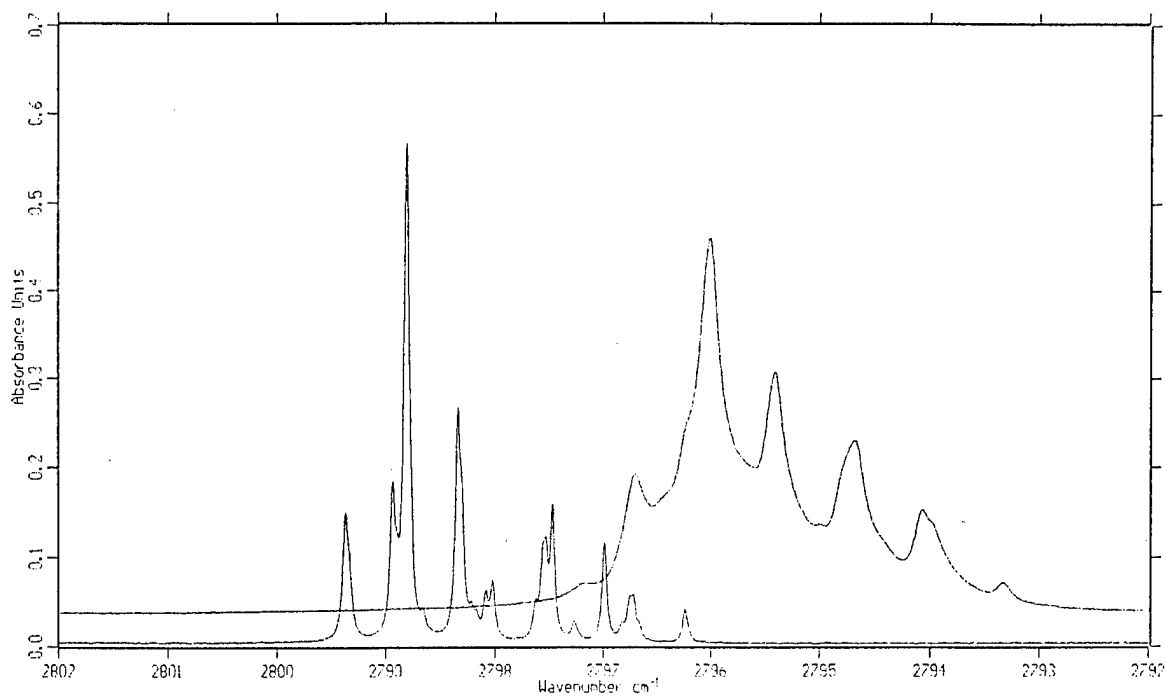
ST28079.1

HCl/pH$_2$ vs. HCl/oD$_2$

st28079.7   annealed   T=2.4K   93 PPM HCl/oD$_2$ ($\approx$98%)
st27061.11 annealed   T=2.4K   88 PPM HCl/pH2 (99.99+%)

ST27061.11

(HCl)$_3$/pH$_2$ & (HCl)$_3$/oD$_2$

st28079.7   annealed   T=2.4K   93 PPM HCl/oD$_2$ (≈98%)
st27061.11 annealed   T=2.4K   88 PPM HCl/pH2 (99.99+%)

ST27061.11

^{13}C^{18}O/pH$_2$ d≈3mm

st28082.6   annealed   T=2.4K
st28082.4   annealing   T=4.8K
st28082.2   as deposited T=2.4K   11 PPM ^{13}CO/pH$_2$ resolution = 0.005 cm^{-1}